

Search history

Nwaonicha 10/521377

05/26/2006

=> d his full

(FILE 'HOME' ENTERED AT 13:31:33 ON 26 MAY 2006)

FILE 'STNGUIDE' ENTERED AT 13:31:55 ON 26 MAY 2006

FILE 'REGISTRY' ENTERED AT 13:32:50 ON 26 MAY 2006

FILE 'STNGUIDE' ENTERED AT 13:33:31 ON 26 MAY 2006

SET LINE 250
SET DETAIL OFF
DIS SAVED/S
SET LINE LOGIN
SET DETAIL LOGIN

FILE 'HCAPLUS' ENTERED AT 13:34:25 ON 26 MAY 2006

ACT NWA377APP/A

L1 1 SEA ABB=ON PLU=ON US2005-521377 /APPS

FILE 'REGISTRY' ENTERED AT 13:34:38 ON 26 MAY 2006

ACT NWA377RNS/A

L2 5 SEA ABB=ON PLU=ON (10605-40-0/BI OR 1066-35-9/BI OR 107-05-1/
BI OR 111-78-4/BI OR 12112-67-3/BI)

ACT NWA377IR/A

L3 47943 SEA ABB=ON PLU=ON IR>0

ACT NWA377IR2/A

L4 7579 SEA ABB=ON PLU=ON IR>1

ACT NWA377BATCH/A

L5 STR

L6 428852 SEA SSS FUL L5

FILE 'HCAPLUS' ENTERED AT 13:37:55 ON 26 MAY 2006

ACT NWA377IR2CAT/A

L7 (7579)SEA ABB=ON PLU=ON IR>1

L8 725 SEA ABB=ON PLU=ON L7/CAT

FILE 'STNGUIDE' ENTERED AT 13:38:08 ON 26 MAY 2006

FILE 'HCAPLUS' ENTERED AT 13:39:45 ON 26 MAY 2006

FILE 'STNGUIDE' ENTERED AT 13:40:08 ON 26 MAY 2006

FILE 'REGISTRY' ENTERED AT 13:42:50 ON 26 MAY 2006

L9 STRUCTURE UPLOADED

L10 50 SEA SUB=L6 SSS SAM L9

L11 424806 SEA SUB=L6 SSS FUL L9

DELETE DAV244PSTRA/A
DELETE DAV244PSTRP/A

DELETE DAV244PSTRQ/A
DELETE OWE120AOLD/A
DELETE OWE120NOTOLD/A
DELETE OWE120UBIQ/A

FILE 'STNGUIDE' ENTERED AT 13:47:26 ON 26 MAY 2006

FILE 'REGISTRY' ENTERED AT 14:25:23 ON 26 MAY 2006

L12 4046 SEA ABB=ON PLU=ON L6 NOT L11

FILE 'HCAPLUS' ENTERED AT 14:26:04 ON 26 MAY 2006

L13 2857503 SEA ABB=ON PLU=ON (RACT OR RCT OR RGT)/RL

L*** DEL 683 S L13 AND L8

FILE 'STNGUIDE' ENTERED AT 14:29:52 ON 26 MAY 2006

FILE 'STNGUIDE' ENTERED AT 14:31:27 ON 26 MAY 2006

FILE 'REGISTRY' ENTERED AT 14:32:00 ON 26 MAY 2006

L14 STRUCTURE UPLOADED

L15 12 SEA SUB=L6 SSS SAM L14

L16 5231 SEA SUB=L6 SSS FUL L14

SAVE TEMP L16 NWA377STRD/A

FILE 'HCAPLUS' ENTERED AT 14:34:16 ON 26 MAY 2006

L17 9286 SEA ABB=ON PLU=ON L16 (L) L13

L18 39 SEA ABB=ON PLU=ON L17 AND L8

SEL RN L18

FILE 'REGISTRY' ENTERED AT 14:36:32 ON 26 MAY 2006

L19 837 SEA ABB=ON PLU=ON (12112-67-3/BI OR 617-86-7/BI OR 1066-35-9/
BI OR 107-05-1/BI OR 766-77-8/BI OR 10605-40-0/BI OR 18827-81-1
/BI OR 603-35-0/BI OR 998-30-1/BI OR 29681-57-0/BI OR 7440-05-3
/BI OR 7440-06-4/BI OR 111-78-4/BI OR 12246-51-4/BI OR
15243-33-1/BI OR 108-94-1/BI OR 12092-47-6/BI OR 14694-95-2/BI
OR 2031-62-1/BI OR 2487-90-3/BI OR 592-41-6/BI OR 7440-18-8/BI
OR 789-25-3/BI OR 98-86-2/BI OR 100-42-5/BI OR 100-52-7/BI OR
10210-68-1/BI OR 1079-66-9/BI OR 12111-11-4/BI OR 12148-71-9/BI
OR 13938-94-8/BI OR 14857-34-2/BI OR 16941-92-7/BI OR
4342-22-7/BI OR 498-66-8/BI OR 536-74-3/BI OR 603-32-7/BI OR
64-17-5/BI OR 693-02-7/BI OR 7439-88-5/BI OR 7440-04-2/BI OR
776-76-1/BI OR 930-68-7/BI OR 10025-78-2/BI OR 10170-69-1/BI
OR 1038-95-5/BI OR 104-53-0/BI OR 106-95-6/BI OR 1081-97-6/BI
OR 109-89-7/BI OR 110-54-3/BI OR 1192-62-7/BI OR 12080-32-9/BI
OR 12245-73-7/BI OR 123-72-8/BI OR 13269-52-8/BI OR 13829-48-6/
BI OR 13829-50-0/BI OR 14221-01-3/BI OR 1438-82-0/BI OR
1445-91-6/BI OR 146139-33-5/BI OR 14871-41-1/BI OR 148991-61-1/
BI OR 14996-61-3/BI OR 1517-69-7/BI OR 15696-40-9/BI OR
16941-12-1/BI OR 17685-52-8/BI OR 17718-70-6/BI OR 21693-13-0/B
I OR 220800-76-0/BI OR 220800-77-1/BI OR 220800-78-2/BI OR
220800-79-3/BI OR 24636-31-5/BI OR 2530-87-2/BI OR 25360-32-1/B
I OR 28407-51-4/BI OR 4041-09-2/BI OR 4050-45-7/BI OR 4131-43-5
/BI OR 4547-10-8/BI OR 502-42-1/BI OR 502-49-8/BI OR 5089-70-3/
BI OR 51440-16-5/BI OR 51440-17-6/BI OR 563-80-4/BI OR
565-80-0/BI OR 583-60-8/BI OR 60255-04-1/BI OR 60255-25-6/BI
OR 60255-27-8/BI OR 603-36-1/BI OR 6163-58-2/BI OR 617-35-6/BI
OR 62791-22-4/BI OR 65335-74-2/BI OR 656240-93-6/BI OR
656240-94-7/BI OR 656240-95-8/BI OR 656240-96-9/BI OR 67-64-1/B
I OR 74-85-1/BI OR 75-03-6/BI OR 75-64-9/BI OR 75-78-5/BI OR
75-97-8/BI OR 7553-56-2/BI OR 75573-29-4/

L20 222 SEA ABB=ON PLU=ON L19 AND L11

FILE 'HCAPLUS' ENTERED AT 14:38:23 ON 26 MAY 2006

L21 2871 SEA ABB=ON PLU=ON L20 (L) PREP/RL

L22 32 SEA ABB=ON PLU=ON L18 AND L21

L23 405200 SEA ABB=ON PLU=ON (?ALKENE? OR ?DIENE?)/BI

L24 19 SEA ABB=ON PLU=ON L22 AND L23

L*** DEL 44857 S (SINGLE STEP?)/BI OR (ONE STEP?)/BI OR (1 STEP)/BI

L25 793758 SEA ABB=ON PLU=ON CONTINU?/BI

L26 2 SEA ABB=ON PLU=ON L22 AND L25

FILE 'CASREACT' ENTERED AT 14:44:42 ON 26 MAY 2006

L27 334 SEA ABB=ON PLU=ON L4/CAT
D COST

FILE 'STNGUIDE' ENTERED AT 14:45:43 ON 26 MAY 2006

FILE 'CASREACT' ENTERED AT 14:51:01 ON 26 MAY 2006

L28 5265 SEA ABB=ON PLU=ON L16/RRRT

L29 24 SEA ABB=ON PLU=ON L28 (L) L27

FILE 'HCAPLUS' ENTERED AT 14:52:59 ON 26 MAY 2006

FILE 'REGISTRY' ENTERED AT 14:53:25 ON 26 MAY 2006

L30 3438 SEA ABB=ON PLU=ON L4 AND X>0

FILE 'HCAPLUS' ENTERED AT 14:53:44 ON 26 MAY 2006

L31 517 SEA ABB=ON PLU=ON L30 (L) CAT/RL

L*** DEL 0 S L17 (L) L31

L32 23 SEA ABB=ON PLU=ON L17 AND L31 AND L21

FILE 'STNGUIDE' ENTERED AT 14:57:10 ON 26 MAY 2006

FILE 'REGISTRY' ENTERED AT 14:57:38 ON 26 MAY 2006

L33 165275 SEA ABB=ON PLU=ON L11 AND CASREACT/LC

FILE 'STNGUIDE' ENTERED AT 14:58:44 ON 26 MAY 2006

FILE 'REGISTRY' ENTERED AT 15:02:04 ON 26 MAY 2006

L34 STRUCTURE UPLOADED

L35 50 SEA SUB=L6 SSS SAM L34

FILE 'STNGUIDE' ENTERED AT 15:03:11 ON 26 MAY 2006

FILE 'CASREACT' ENTERED AT 15:04:44 ON 26 MAY 2006

FILE 'STNGUIDE' ENTERED AT 15:05:10 ON 26 MAY 2006

FILE 'CASREACT' ENTERED AT 15:07:34 ON 26 MAY 2006

L36 STRUCTURE UPLOADED

L37 29 SEA SSS SAM L36 (1513 REACTIONS)

FILE 'STNGUIDE' ENTERED AT 15:08:14 ON 26 MAY 2006

FILE 'CASREACT' ENTERED AT 15:12:09 ON 26 MAY 2006

L38 STRUCTURE UPLOADED

L39 4 SEA SSS SAM L38 (49 REACTIONS)
D STAT QUE L37
D STAT QUE L39

L40 STRUCTURE UPLOADED

L41 4 SEA SSS SAM L40 (37 REACTIONS)

FILE 'STNGUIDE' ENTERED AT 15:17:01 ON 26 MAY 2006
D SCA

FILE 'HCAPLUS' ENTERED AT 15:18:04 ON 26 MAY 2006

L42 24 SEA ABB=ON PLU=ON L29
L43 16 SEA ABB=ON PLU=ON L22 AND L42
L44 12 SEA ABB=ON PLU=ON L32 AND L42

FILE 'CASREACT' ENTERED AT 15:20:56 ON 26 MAY 2006

D SCA L29
SEL RX L29
DELETE SELECT
SEL RX L29

FILE 'REGISTRY' ENTERED AT 15:29:43 ON 26 MAY 2006

EDIT E1-E262 RX RN
L45 262 SEA ABB=ON PLU=ON (75-09-2/RN OR 7732-18-5/RN OR 107-06-2/RN
OR 12112-67-3/RN OR 109-99-9/RN OR 110-54-3/RN OR 67-56-1/RN
OR 617-86-7/RN OR 760-32-7/RN OR 501419-01-8/RN OR 144-55-8/RN
OR 501419-19-8/RN OR 501419-20-1/RN OR 501419-21-2/RN OR
603-35-0/RN OR 501419-22-3/RN OR 75-05-8/RN OR 108-48-5/RN OR
12246-51-4/RN OR 501419-23-4/RN OR 69739-34-0/RN OR 185346-09-2
/RN OR 96-33-3/RN OR 501419-02-9/RN OR 18827-81-1/RN OR
501419-08-5/RN OR 501419-27-8/RN OR 7647-01-0/RN OR 1191-15-7/R
N OR 121289-23-4/RN OR 501419-10-9/RN OR 304-59-6/RN OR
501419-28-9/RN OR 108-94-1/RN OR 87413-09-0/RN OR 108-88-3/RN
OR 501419-29-0/RN OR 558-13-4/RN OR 60-29-7/RN OR 74-88-4/RN
OR 109-72-8/RN OR 12125-02-9/RN OR 584-08-7/RN OR 37342-97-5/RN
OR 56-23-5/RN OR 7553-56-2/RN OR 14221-01-3/RN OR 501419-06-3/
RN OR 594-19-4/RN OR 7646-85-7/RN OR 1066-35-9/RN OR 1333-74-0/
RN OR 429-41-4/RN OR 4342-22-7/RN OR 10605-40-0/RN OR 109389-69
-7/RN OR 13810-04-3/RN OR 82499-43-2/RN OR 107-05-1/RN OR
12148-71-9/RN OR 29681-57-0/RN OR 501419-32-5/RN OR 592-41-6/RN
OR 762-42-5/RN OR 930-68-7/RN OR 4419-18-5/RN OR 616-47-7/RN
OR 630-08-0/RN OR 84-58-2/RN OR 96474-45-2/RN OR 101-02-0/RN
OR 121-44-8/RN OR 124-63-0/RN OR 501419-33-6/RN OR 111-78-4/RN
OR 123-91-1/RN OR 603-32-7/RN OR 71195-85-2/RN OR 7664-39-3/RN
OR 109-89-7/RN OR 501419-34-7/RN OR 64-17-5/RN OR 70790-00-0/RN
OR 75-03-6/RN OR 110-82-7/RN OR 151-50-8/RN OR 168557-46-8/RN
OR 513-81-5/RN OR 598-30-1/RN OR 7782-44-7/RN OR 107-30-2/RN
OR 111-66-0/RN OR 13508-63-9/RN OR 168557-50-4/RN OR 168557-53-
7/RN OR 2227-29-4/RN OR 40962-02-5/RN OR 501419-30-3/RN OR
57-14-7/RN OR 627-19-0/RN OR 68928-07-4/RN OR 68928-08-5/RN OR
7087-68-5/RN OR 998-30-1/RN OR 100-42-5/RN OR 100-52-7/RN OR
10175-53-8/RN OR 1192-62-7/RN OR 123-72-8/RN OR 162157-02-0/RN
OR 168557-47-9/RN OR

FILE 'CASREACT' ENTERED AT 15:31:34 ON 26 MAY 2006

L46 12591 SEA ABB=ON PLU=ON L45/PRO
L47 24 SEA ABB=ON PLU=ON L29 (L) L46

FILE 'HCAPLUS' ENTERED AT 15:34:40 ON 26 MAY 2006

FILE 'STNGUIDE' ENTERED AT 15:34:55 ON 26 MAY 2006

FILE 'HCAPLUS' ENTERED AT 15:36:42 ON 26 MAY 2006

L48 1 SEA ABB=ON PLU=ON L1 AND L22
L49 12 SEA ABB=ON PLU=ON KORNEK T?/AU

L50 1132 SEA ABB=ON PLU=ON BAUER A?/AU
L51 1 SEA ABB=ON PLU=ON SENDEN D?/AU
L52 1 SEA ABB=ON PLU=ON (L49 AND (L50 OR L51)) OR (L50 AND L51)
L53 2 SEA ABB=ON PLU=ON (L49 OR L50 OR L51) AND (L22 OR L24 OR L26
OR L32)

FILE 'CASREACT' ENTERED AT 15:38:22 ON 26 MAY 2006

L54 8 SEA ABB=ON PLU=ON KORNEK T?/AU
L55 33 SEA ABB=ON PLU=ON BAUER A?/AU
L56 1 SEA ABB=ON PLU=ON SENDEN D?/AU
L57 1 SEA ABB=ON PLU=ON (L54 AND (L55 OR L56)) OR (L55 AND L56)
L58 2 SEA ABB=ON PLU=ON (L54 OR L55 OR L56) AND L47

FILE 'STNGUIDE' ENTERED AT 15:40:40 ON 26 MAY 2006

FILE 'REGISTRY' ENTERED AT 15:44:49 ON 26 MAY 2006

D STAT QUE L6
D STAT QUE L11
D STAT QUE L16

FILE 'HCAPLUS' ENTERED AT 15:45:34 ON 26 MAY 2006

D QUE NOS L52
D QUE NOS L53
L59 2 SEA ABB=ON PLU=ON L52 OR L53

FILE 'CASREACT' ENTERED AT 15:46:49 ON 26 MAY 2006

D QUE NOS L57
D QUE NOS L58
L60 2 SEA ABB=ON PLU=ON L57 OR L58

FILE 'HCAPLUS, CASREACT' ENTERED AT 15:47:25 ON 26 MAY 2006

L61 2 DUP REM L59 L60 (2 DUPLICATES REMOVED)
ANSWERS '1-2' FROM FILE HCAPLUS
D IBIB ABS HITIND HITSTR L61 1-2

FILE 'STNGUIDE' ENTERED AT 15:48:20 ON 26 MAY 2006

FILE 'CASREACT' ENTERED AT 15:50:26 ON 26 MAY 2006

D QUE NOS L47
L62 22 SEA ABB=ON PLU=ON L47 NOT L60

FILE 'HCAPLUS' ENTERED AT 15:50:30 ON 26 MAY 2006

D QUE NOS L22
D QUE NOS L24
D QUE NOS L26
D QUE NOS L32
L63 30 SEA ABB=ON PLU=ON (L22 OR L24 OR L26 OR L32) NOT L59

FILE 'CASREACT, HCAPLUS' ENTERED AT 15:50:58 ON 26 MAY 2006

L64 38 DUP REM L62 L63 (14 DUPLICATES REMOVED)
ANSWERS '1-22' FROM FILE CASREACT
ANSWERS '23-38' FROM FILE HCAPLUS
D IBIB ABS HIT L64 1-22
D IBIB ABS HITIND HITSTR L64 23-38

FILE HOME

FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: May 19, 2006 (20060519/UP).

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 MAY 2006 HIGHEST RN 885654-58-0

DICTIONARY FILE UPDATES: 25 MAY 2006 HIGHEST RN 885654-58-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

FILE HCAPLUS

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FILE COVERS 1907 - 26 May 2006 VOL 144 ISS 23

FILE LAST UPDATED: 25 May 2006 (20060525/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE CASREACT

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FILE CONTENT:1840 - 21 May 2006 VOL 144 ISS 21

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*
* CASREACT now has more than 10 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

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=> file_registry

FILE 'REGISTRY' ENTERED AT 15:44:49 ON 26 MAY 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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STRUCTURE FILE UPDATES: 25 MAY 2006 HIGHEST RN 885654-58-0
DICTIONARY FILE UPDATES: 25 MAY 2006 HIGHEST RN 885654-58-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

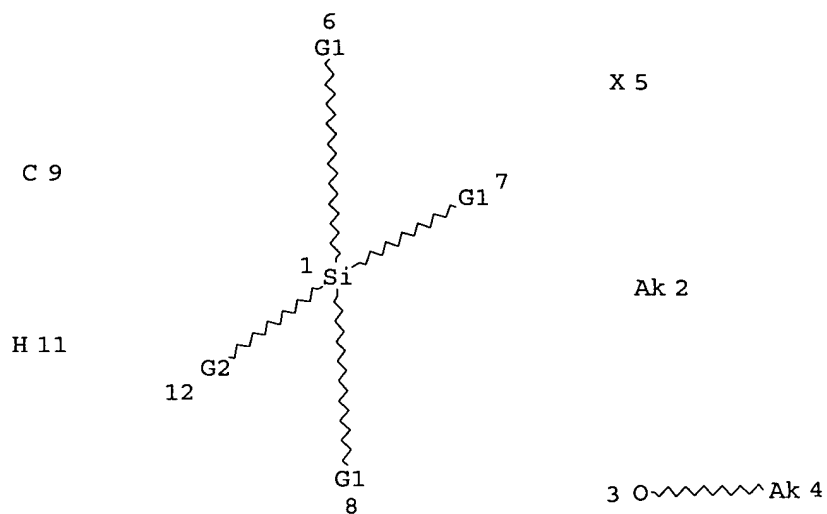
<http://www.cas.org/ONLINE/UG/regprops.html>

=> d stat que L6

L5 STR

STRUCTURE
QUERIES

C 10



VAR G1=2/3/5

VAR G2=9/10/11

NODE ATTRIBUTES:

NSPEC	IS C	AT	1
NSPEC	IS C	AT	2
NSPEC	IS C	AT	3
NSPEC	IS C	AT	4
NSPEC	IS C	AT	5
NSPEC	IS C	AT	6
NSPEC	IS C	AT	7
NSPEC	IS C	AT	8
NSPEC	IS C	AT	9
NSPEC	IS R	AT	10
NSPEC	IS C	AT	11
NSPEC	IS C	AT	12

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 1 2 3 4 5 9 11

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L6 428852 SEA FILE=REGISTRY SSS FUL L5

100.0% PROCESSED 1236316 ITERATIONS

428852 ANSWERS

SEARCH TIME: 00.00.12

=> d stat que L11

L5 STR

=> □

CASREACT 1-22; HCAPIUS 23-38

=> file casreact

FILE=CASREACT ENTERED AT 15:50:26 ON 26 MAY 2006
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FILE CONTENT:1840 - 21 May 2006 VOL 144 ISS 21

New CAS Information Use Policies, enter HELP USAGETERMS for details.

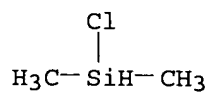
* CASREACT now has more than 10 million reactions *
* *****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

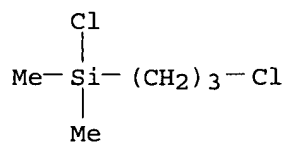
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que nos L47

L4 7579 SEA FILE=REGISTRY ABB=ON PLU=ON IR>1
L5 STR
L6 428852 SEA FILE=REGISTRY SSS FUL L5
L14 STR
L16 5231 SEA FILE=REGISTRY SUB=L6 SSS FUL L14
L27 334 SEA FILE=CASREACT ABB=ON PLU=ON L4/CAT
L28 5265 SEA FILE=CASREACT ABB=ON PLU=ON L16/RRT
L29 24 SEA FILE=CASREACT ABB=ON PLU=ON L28 (L) L27
L45 262 SEA FILE=REGISTRY ABB=ON PLU=ON (75-09-2/RN OR 7732-18-5/RN
OR 107-06-2/RN OR 12112-67-3/RN OR 109-99-9/RN OR 110-54-3/RN
OR 67-56-1/RN OR 617-86-7/RN OR 760-32-7/RN OR 501419-01-8/RN
OR 144-55-8/RN OR 501419-19-8/RN OR 501419-20-1/RN OR 501419-21
-2/RN OR 603-35-0/RN OR 501419-22-3/RN OR 75-05-8/RN OR
108-48-5/RN OR 12246-51-4/RN OR 501419-23-4/RN OR 69739-34-0/RN
OR 185346-09-2/RN OR 96-33-3/RN OR 501419-02-9/RN OR 18827-81-
1/RN OR 501419-08-5/RN OR 501419-27-8/RN OR 7647-01-0/RN OR
1191-15-7/RN OR 121289-23-4/RN OR 501419-10-9/RN OR 304-59-6/RN
OR 501419-28-9/RN OR 108-94-1/RN OR 87413-09-0/RN OR 108-88-3/
RN OR 501419-29-0/RN OR 558-13-4/RN OR 60-29-7/RN OR 74-88-4/RN
OR 109-72-8/RN OR 12125-02-9/RN OR 584-08-7/RN OR 37342-97-5/R
N OR 56-23-5/RN OR 7553-56-2/RN OR 14221-01-3/RN OR 501419-06-3
/RN OR 594-19-4/RN OR 7646-85-7/RN OR 1066-35-9/RN OR 1333-74-0
/RN OR 429-41-4/RN OR 4342-22-7/RN OR 10605-40-0/RN OR
109389-69-7/RN OR 13810-04-3/RN OR 82499-43-2/RN OR 107-05-1/RN
OR 12148-71-9/RN OR 29681-57-0/RN OR 501419-32-5/RN OR
592-41-6/RN OR 762-42-5/RN OR 930-68-7/RN OR 4419-18-5/RN OR
616-47-7/RN OR 630-08-0/RN OR 84-58-2/RN OR 96474-45-2/RN OR
101-02-0/RN OR 121-44-8/RN OR 124-63-0/RN OR 501419-33-6/RN OR

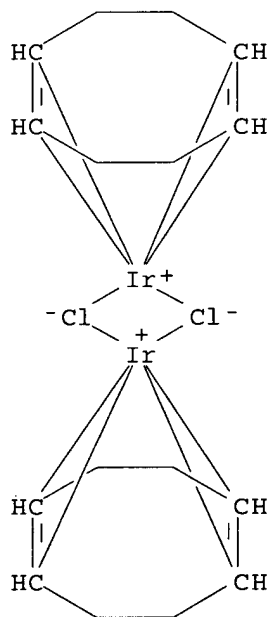


IT 10605-40-0P, Chloro(3-chloropropyl)dimethylsilane
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 10605-40-0 HCAPLUS
CN Silane, chloro(3-chloropropyl)dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX
NAME)



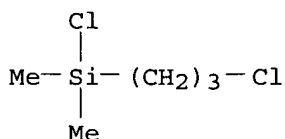
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

CC 29-6 (Organometallic and Organometalloidal Compounds)
 ST organo silane prepn; iridium catalyzed hydrosilylation **alkene**
 hydrosilane; platinum catalyzed hydrosilylation **alkene**
 hydrosilane
 IT Hydrosilylation catalysts
 (preparation of organosilanes via **diene** iridium chloride catalyzed
 hydrosilylation of **alkenes** with hydrosilanes)
 IT 12112-67-3 134588-15-1
 RL: CAT (Catalyst use); USES (Uses)
 (hydrosilylation of allyl chloride with chlorodimethylsilane catalyzed
 with)
 IT 1066-35-9, Chlorodimethylsilane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (iridium catalyzed hydrosilylation of allyl chloride with)
 IT 111-78-4, 1,5-Cyclooctadiene
 RL: CAT (Catalyst use); USES (Uses)
 (iridium catalyzed hydrosilylation of allyl chloride with
 chlorodimethylsilane in presence of)
 IT 10605-40-0P, Chloro(3-chloropropyl)dimethylsilane
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 12112-67-3
 RL: CAT (Catalyst use); USES (Uses)
 (hydrosilylation of allyl chloride with chlorodimethylsilane catalyzed
 with)
 RN 12112-67-3 HCAPLUS
 CN Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di- (9CI)
 (CA INDEX NAME)



IT 1066-35-9, Chlorodimethylsilane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (iridium catalyzed hydrosilylation of allyl chloride with)
 RN 1066-35-9 HCAPLUS
 CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

IT 10605-40-0P, Chloro(3-chloropropyl)dimethylsilane
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (continuous preparation of organosilanes via iridium catalyzed
 reaction of **alkene** with silane)
 RN 10605-40-0 HCAPLUS
 CN Silane, chloro(3-chloropropyl)dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX
 NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L61 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2
 ACCESSION NUMBER: 2002:51103 HCAPLUS
 DOCUMENT NUMBER: 136:102512
 TITLE: Preparation of organosilanes via transition metal
 catalyzed hydrosilylation of **alkenes**
 INVENTOR(S): Schaefer, Oliver; Frey, Volker; Pachaly, Bernd;
Bauer, Andreas; Kriegbaum, Markus; Brader,
 Leonhard
 PATENT ASSIGNEE(S): Consortium fuer Elektrochemische Industrie GmbH,
 Germany
 SOURCE: Ger., 4 pp.
 CODEN: GWXXAW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10053037	C1	20020117	DE 2000-10053037	20001026
EP 1201671	A1	20020502	EP 2001-118869	20010816
EP 1201671	B1	20031112		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2002052520	A1	20020502	US 2001-966822	20010927
US 6388119	B2	20020514		
JP 2002179684	A2	20020626	JP 2001-324905	20011023
CN 1351015	A	20020529	CN 2001-136677	20011024
PRIORITY APPLN. INFO.:			DE 2000-10053037	A 20001026

OTHER SOURCE(S): CASREACT 136:102512; MARPAT 136:102512

AB The preparation of organosilanes, R₆R₅CHCHR₄SiR₁R₂R₃ (R₁-R₃ = Si-C bonded halo
 substituted C₁-18 hydrocarbon, Cl, C₁-18 alkoxy, etc.; R₄-R₆ = H, F, Cl,
 alkoxy, organoamino, CN, NCO substituted C₁-18 hydrocarbon, chloro-,
 fluoro-C₁-18 alkoxy, cyclic, etc.), via [(**diene**)IrCl]₂-catalyzed
 hydrosilylation of R₅R₆CH:CHR₄ with HSiR₁R₂R₃, is described. Thus,
 di-μ-chlorobis[(**cyclooctadiene**)iridium]/1,5-
cyclooctadiene-catalyzed hydrosilylation of allyl chloride with
 chlorodimethylsilane gave 95% chloro(3-chloropropyl)dimethylsilane.

IC ICM C07F007-12
 ICS C07F007-08; C07F007-10; C07F007-18

(organo-; **continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)

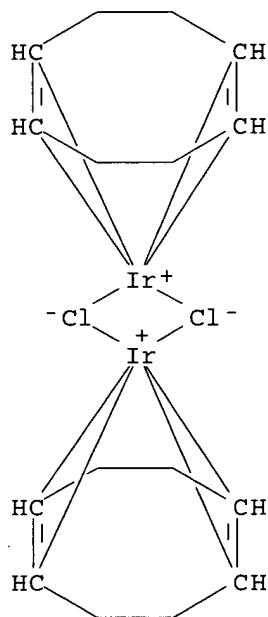
IT 111-78-4, 1,5-Cyclooctadiene 12112-67-3,
Bis[chloro(1,5-cyclooctadiene)iridium]
RL: **CAT (Catalyst use)**; **USES (Uses)**
(**continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)

IT 107-05-1, Allyl chloride 1066-35-9, Chlorodimethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(**continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)

IT 10605-40-0P, Chloro(3-chloropropyl)dimethylsilane
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(**continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)

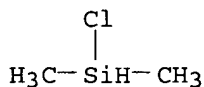
IT 12112-67-3, Bis[chloro(1,5-cyclooctadiene)iridium]
RL: **CAT (Catalyst use)**; **USES (Uses)**
(**continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)

RN 12112-67-3 HCAPLUS
CN Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di- (9CI)
(CA INDEX NAME)



IT 1066-35-9, Chlorodimethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(**continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)

RN 1066-35-9 HCAPLUS
CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



PROCESSING COMPLETED FOR L60

L61 2 DUP REM L59 L60 (2 DUPLICATES REMOVED)

ANSWERS '1-2' FROM FILE HCAPLUS

=> d ibib abs hitind hitstr L61 1-2

L61 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 1

ACCESSION NUMBER: 2003:811648 HCAPLUS

DOCUMENT NUMBER: 139:292356

TITLE: **Continuous** preparation of organosilanes via
iridium catalyzed reaction of **alkene** with
silaneINVENTOR(S): **Kornek, Thomas; Bauer, Andreas;**
Senden, Diana

PATENT ASSIGNEE(S): Wacker-Chemie GmbH, Germany

SOURCE: Ger., 4 pp.

CODEN: GWXXAW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10232663	C1	20031016	DE 2002-10232663	20020718
WO 2004009607	A1	20040129	WO 2003-EP6204	20030612
W: CN, JP, PL, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
EP 1530575	A1	20050518	EP 2003-735613	20030612
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1668624	A	20050914	CN 2003-817180	20030612
JP 2005533123	T2	20051104	JP 2004-522176	20030612
US 2005240043	A1	20051027	US 2005-521377	20050118
PRIORITY APPLN. INFO.:			DE 2002-10232663	A 20020718
			WO 2003-EP6204	W 20030612

OTHER SOURCE(S): CASREACT 139:292356; MARPAT 139:292356

AB Procedure for the **continuous** production of silane,
R6R5CHR4CHSiR1R2R3 (R1-R3 = C1-18 hydrocarbyl, Cl, C1-18 alkoxy, etc.;
R4-R6 = H, F, Cl, alkoxy, amino, cyano, NCO, C1-18 hydrocarbyl, etc.), via
[(**diene**)IrCl]2-catalyzed reaction of silane HSiR1R2R3 with
alkene R6R5CH:CHR4 and free **diene** as cocatalyst is
described. [(cod)IrCl]2. The reaction temperature 30-200° and the
reaction pressure 0.11-50.0 Mpa.

IC ICM C07F007-12

ICS C07F007-08; C07F007-10; C07F007-18

CC 29-6 (Organometallic and Organometalloidal Compounds)

ST organo silane prepn; iridium **diene** halide catalyzed addn silane
alkene

IT Addition reaction

Addition reaction catalysts

(continuous preparation of organosilanes via iridium catalyzed
reaction of **alkene** with silane)IT **Alkenes**, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(continuous preparation of organosilanes via iridium catalyzed
reaction of **alkene** with silane)

IT Silanes

RL: SPN (Synthetic preparation); PREP (Preparation)

=> d que nos L58

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 L6 428852 SEA FILE=REGISTRY SSS FUL L5
 L14 STR
 L16 5231 SEA FILE=REGISTRY SUB=L6 SSS FUL L14
 L27 334 SEA FILE=CASREACT ABB=ON PLU=ON L4/CAT
 L28 5265 SEA FILE=CASREACT ABB=ON PLU=ON L16/RRT
 L29 24 SEA FILE=CASREACT ABB=ON PLU=ON L28 (L) L27
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 OR 144-55-8/RN OR 501419-19-8/RN OR 501419-20-1/RN OR 501419-21
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 70790-00-0/RN OR 75-03-6/RN OR 110-82-7/RN OR 151-50-8/RN OR
 168557-46-8/RN OR 513-81-5/RN OR 598-30-1/RN OR 7782-44-7/RN
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 OR 100-52-7/RN OR 10175-53-8/RN OR 1192-62-7/RN OR 123-72-8/RN
 OR 162157-02-0/RN OR 168557-47-9/RN OR
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 L47 24 SEA FILE=CASREACT ABB=ON PLU=ON L29 (L) L46
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 L55 33 SEA FILE=CASREACT ABB=ON PLU=ON BAUER A?/AU
 L56 1 SEA FILE=CASREACT ABB=ON PLU=ON SENDEN D?/AU
 L58 2 SEA FILE=CASREACT ABB=ON PLU=ON ~~(L54, OR L55, OR L56) AND L47~~

=> s L57 or L58

L60 2 L57 OR L58

=> dup rem L59 L60

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OR 60255-27-8/BI OR 603-36-1/BI OR 6163-58-2/BI OR 617-35-6/BI
OR 62791-22-4/BI OR 65335-74-2/BI OR 656240-93-6/BI OR
656240-94-7/BI OR 656240-95-8/BI OR 656240-96-9/BI OR 67-64-1/B
I OR 74-85-1/BI OR 75-03-6/BI OR 75-64-9/BI OR 75-78-5/BI OR
75-97-8/BI OR 7553-56-2/BI OR 75573-29-4/

L20 222 SEA FILE=REGISTRY ABB=ON PLU=ON L19 AND L11
L21 2871 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 (L) PREP/RL
L22 32 SEA FILE=HCAPLUS ABB=ON PLU=ON L18 AND L21
L23 405200 SEA FILE=HCAPLUS ABB=ON PLU=ON (?ALKENE? OR ?DIENE?)/BI
L24 19 SEA FILE=HCAPLUS ABB=ON PLU=ON L22 AND L23
L25 793758 SEA FILE=HCAPLUS ABB=ON PLU=ON CONTINU?/BI
L26 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L22 AND L25
L30 3438 SEA FILE=REGISTRY ABB=ON PLU=ON L4 AND X>0
L31 517 SEA FILE=HCAPLUS ABB=ON PLU=ON L30 (L) CAT/RL
L32 23 SEA FILE=HCAPLUS ABB=ON PLU=ON L17 AND L31 AND L21
L49 12 SEA FILE=HCAPLUS ABB=ON PLU=ON KORNEK T?/AU
L50 1132 SEA FILE=HCAPLUS ABB=ON PLU=ON BAUER A?/AU
L51 1 SEA FILE=HCAPLUS ABB=ON PLU=ON SENDEN D?/AU
L53 2 SEA FILE=HCAPLUS ABB=ON PLU=ON (L49 OR L50 OR L51) AND (L22
OR L24 OR L26 OR L32)

=> s L52 or L53

L59 2 L52 OR L53

=> file casreact

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FILE CONTENT:1840 - 21 May 2006 VOL 144 ISS 21

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que nos L57

L54 8 SEA FILE=CASREACT ABB=ON PLU=ON KORNEK T?/AU
L55 33 SEA FILE=CASREACT ABB=ON PLU=ON BAUER A?/AU
L56 1 SEA FILE=CASREACT ABB=ON PLU=ON SENDEN D?/AU
L57 1 SEA FILE=CASREACT ABB=ON PLU=ON (L54 AND (L55 OR L56)) OR
(L55 AND L56)

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FILE COVERS 1907 - 26 May 2006 VOL 144 ISS 23
FILE LAST UPDATED: 25 May 2006 (20060525/ED)

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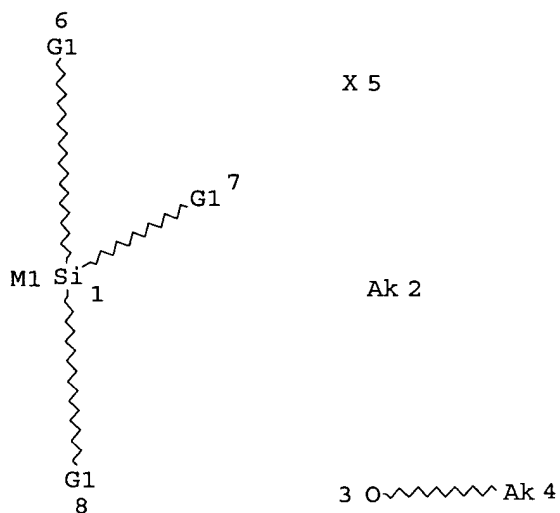
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L51 1 SEA FILE=HCAPLUS ABB=ON PLU=ON SENDEN D?/AU
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(L50 AND L51)

=> d que nos L53

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L13 2857503 SEA FILE=HCAPLUS ABB=ON PLU=ON (RACT OR RCT OR RGT)/RL
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VAR G1=2/3/5

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DEFAULT ECLEVEL IS LIMITED			

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L16 5231 SEA FILE=REGISTRY SUB=L6 SSS FUL L14

100.0% PROCESSED 428849 ITERATIONS
SEARCH TIME: 00.00.05

5231 ANSWERS

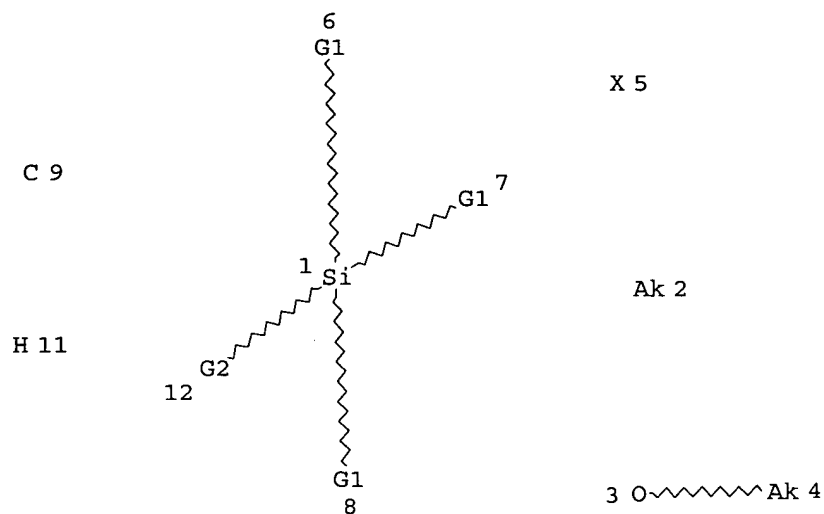
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C 10



VAR G1=2/3/5

VAR G2=9/10/11

NODE ATTRIBUTES:

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DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 1 2 3 4 5 9 11

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

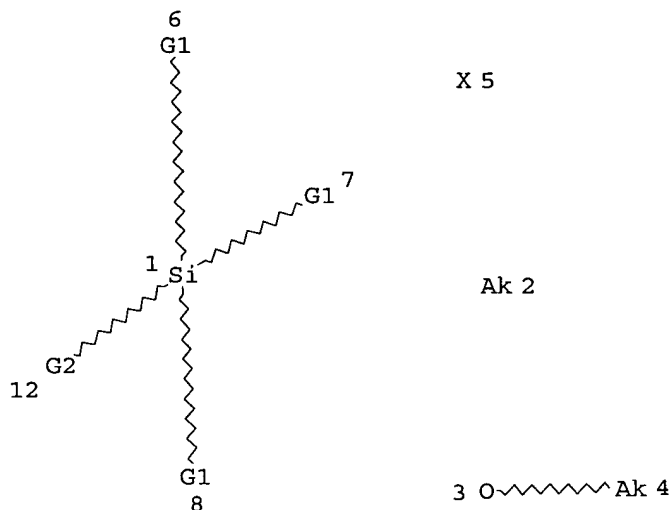
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L14 STR

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C 9

H 11



VAR G1=2/3/5

VAR G2=9/10/11

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NSPEC	IS C	AT	4
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NSPEC	IS C	AT	6
NSPEC	IS C	AT	7
NSPEC	IS C	AT	8
NSPEC	IS C	AT	9
NSPEC	IS R	AT	10
NSPEC	IS C	AT	11
NSPEC	IS C	AT	12

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 1 2 3 4 5 9 11

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L6 428852 SEA FILE=REGISTRY SSS FUL L5

L9 STR

L11 424806 SEA FILE=REGISTRY SUB=L6 SSS FUL L9

100.0% PROCESSED 428456 ITERATIONS

424806 ANSWERS

SEARCH TIME: 00.00.05

=> d stat que L16

L5

STR

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 7664-39-3/RN OR 109-89-7/RN OR 501419-34-7/RN OR 64-17-5/RN OR
 70790-00-0/RN OR 75-03-6/RN OR 110-82-7/RN OR 151-50-8/RN OR
 168557-46-8/RN OR 513-81-5/RN OR 598-30-1/RN OR 7782-44-7/RN
 OR 107-30-2/RN OR 111-66-0/RN OR 13508-63-9/RN OR 168557-50-4/R
 N OR 168557-53-7/RN OR 2227-29-4/RN OR 40962-02-5/RN OR
 501419-30-3/RN OR 57-14-7/RN OR 627-19-0/RN OR 68928-07-4/RN
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 OR 100-52-7/RN OR 10175-53-8/RN OR 1192-62-7/RN OR 123-72-8/RN
 OR 162157-02-0/RN OR 168557-47-9/RN OR

L46 12591 SEA FILE=CASREACT ABB=ON PLU=ON L45/PRO

L47 24 SEA FILE=CASREACT ABB=ON PLU=ON L29 (L) L46

=> s L47 not L60

L62 22 L47 NOT L60

=> file hcaplus

FILE 'HCAPLUS' ENTERED AT 15:50:30 ON 26 MAY 2006

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FILE COVERS 1907 - 26 May 2006 VOL 144 ISS 23

FILE LAST UPDATED: 25 May 2006 (20060525/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

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 L7 (7579) SEA FILE=REGISTRY ABB=ON PLU=ON IR>1
 L8 725 SEA FILE=HCAPLUS ABB=ON PLU=ON L7/CAT
 L9 STR
 L11 424806 SEA FILE=REGISTRY SUB=L6 SSS FUL L9
 L13 2857503 SEA FILE=HCAPLUS ABB=ON PLU=ON (RACT OR RCT OR RGT)/RL
 L14 STR
 L16 5231 SEA FILE=REGISTRY SUB=L6 SSS FUL L14
 L17 9286 SEA FILE=HCAPLUS ABB=ON PLU=ON L16 (L) L13
 L18 39 SEA FILE=HCAPLUS ABB=ON PLU=ON L17 AND L8
 L19 837 SEA FILE=REGISTRY ABB=ON PLU=ON (12112-67-3/BI OR 617-86-7/BI
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 L21 2871 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 (L) PREP/RL
 L22 32 SEA FILE=HCAPLUS ABB=ON PLU=ON L18 AND L21

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 L9 STR
 L11 424806 SEA FILE=REGISTRY SUB=L6 SSS FUL L9
 L13 2857503 SEA FILE=HCAPLUS ABB=ON PLU=ON (RACT OR RCT OR RGT)/RL
 L14 STR
 L16 5231 SEA FILE=REGISTRY SUB=L6 SSS FUL L14
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 L21 2871 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 (L) PREP/RL
 L22 32 SEA FILE=HCAPLUS ABB=ON PLU=ON L18 AND L21
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 L14 STR
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 L22 32 SEA FILE=HCAPLUS ABB=ON PLU=ON L18 AND L21
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 L20 222 SEA FILE=REGISTRY ABB=ON PLU=ON L19 AND L11
 L21 2871 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 (L) PREP/RL
 L30 3438 SEA FILE=REGISTRY ABB=ON PLU=ON L4 AND X>0
 L31 517 SEA FILE=HCAPLUS ABB=ON PLU=ON L30 (L) CAT/RL
 L32 23 SEA FILE=HCAPLUS ABB=ON PLU=ON L17 AND L31 AND L21

=> s (L22 or L24 or L26 or L32) not L59

L63 30 (L22 OR L24 OR L26 OR L32) NOT L59

=> dup rem L62 L63

FILE 'CASREACT' ENTERED AT 15:50:58 ON 26 MAY 2006
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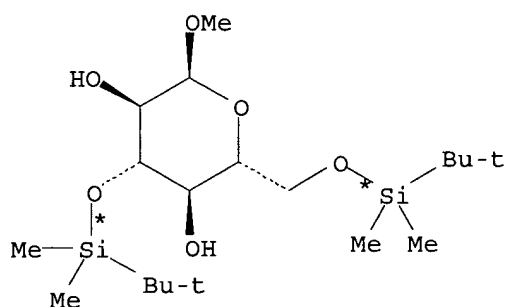
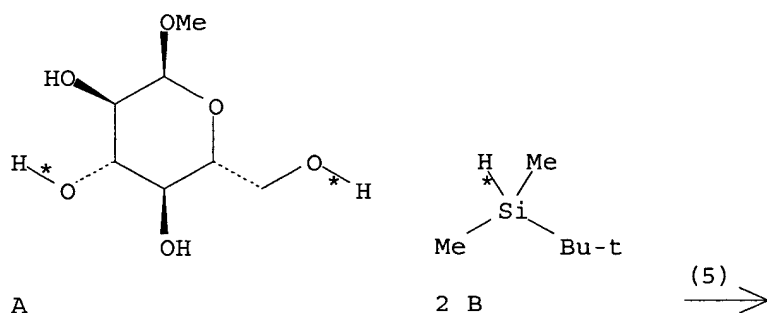
FILE 'HCAPLUS' ENTERED AT 15:50:58 ON 26 MAY 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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PROCESSING COMPLETED FOR L62
PROCESSING COMPLETED FOR L63

L64 38 DUP REM L62 L63 (14 DUPLICATES REMOVED)
ANSWERS '1-22' FROM FILE CASREACT
ANSWERS '23-38' FROM FILE HCAPLUS

=> d ibib abs hit L64 1-22; d ibib abs hitind hitstr L64 23-38

L64 ANSWER 1 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 144:129167 CASREACT
TITLE: Regioselectively Trisilylated Hexopyranosides through Homogeneously Catalyzed Silane Alcoholysis
AUTHOR(S): Chung, Mee-Kyung; Schlaf, Marcel
CORPORATE SOURCE: Guelph-Waterloo Centre for Graduate Work in Chemistry (GWC), Department of Chemistry, University of Guelph, Guelph, ON, N1G 2W1, Can.
SOURCE: Journal of the American Chemical Society (2005), 127(51), 18085-18092
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The iridium complex [Ir(COD)(PPh₃)₂]+SbF₆⁻ reacts with tert-butyldimethylsilane in DMA to form [IrH₂(Sol)₂(PPh₃)₂]+SbF₆⁻, which is an active catalyst for the regioselective di- and trisilylation of a series of representative Me hexopyranosides, β-1,6-anhydrohexopyranosides and 1,3,5-O-methylidene inositol. The corresponding 2,3,6- and 2,4,6-silylated glycosides are obtained in a separable mixture of 47-89% (2,3,6-isomers) and 9-25% (2,4,6-isomers) yield in a single-pot reaction. The 2,4-disilylated derivs. of mannosan, galactosan, and 1,3,5-O-methylidene inositol as well as persilylated levoglucosan are accessible in >85% yield by this method. The homogeneous nature of the catalysts is a prerequisite for the effective di-/trisilylation, as nanoparticle colloid catalysts generated in situ from Pd₂(dba)₃ (.apprx.1.5 nm average particle size) or Ru₂Cl₅(MeCN)₇ (.apprx.0.65 nm average particle size) result in only low yields.
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(5) OF 48 A + 2 B ==> D



YIELD 46%

RX (5) RCT A 97-30-3, B 29681-57-0
 PRO D 68102-62-5
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
 SOL 127-19-5 AcNMe2
 CON SUBSTAGE(1) 15 hours, room temperature
 SUBSTAGE(2) 45 deg C
 NTE other products also detected, regioselective

L64 ANSWER 2 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 142:56520 CASREACT

TITLE: Process for preparation of (haloalkyl)chlorosilanes by hydrosilylation of an alkenyl halide with a halosilane in presence of an iridium catalyst and an auxiliary ketone, ether, quinone, anhydride, unsatd. hydrocarbon or their mixtures

INVENTOR(S): Galland, Jean Christophe; Guennouni, Nathalie

PATENT ASSIGNEE(S): Rhodia Chimie, Fr.

SOURCE: Fr. Demande, 24 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

KIND DATE

APPLICATION NO. DATE

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FR 2856402      A1      20041224      FR 2003-50222      20030617
FR 2856402      B1      20050826
WO 2004113354   A2      20041229      WO 2004-FR1487     20040616
WO 2004113354   A3      20050317

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W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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EP 1633761      A2      20060315      EP 2004-767350     20040616

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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

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PRIORITY APPLN. INFO.:      FR 2003-50222      20030617
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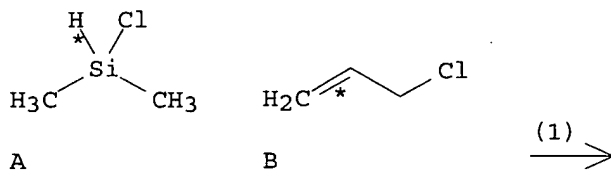
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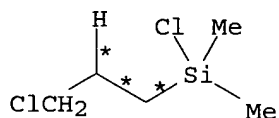
OTHER SOURCE(S): MARPAT 142:56520

AB Dialkyl (halo) (haloalkyl) silanes $\text{XRR}_1\text{Si}(\text{CH}_2)_x\text{X}$ [X = Cl, Br, iodo; x = 2-10; R, R₁ = (un)branched C1-6 alkyl, Ph] are prepared by hydrosilylation of an alkenyl halide $\text{CH}_2\text{:CH}(\text{CH}_2)_x\text{X}$ (same X, x) with a silane XRR_2SiH (same X, R, R₁) in presence of an Ir(I) or Ir(III) catalyst and an (un)supported auxiliary selected from the group of compds. including (i) ketones, (ii) ethers, (iii) quinones, (iv) anhydrides, (v) (a)cyclic C4-30 unsatd. hydrocarbons that are aromatic and/or contain at least one C:C double bond and/or at least one C.tplbond.C triple bond, where these unsatd. bonds may be conjugated, having 1-8 ethylene and/or acetylenic bonds and may have one or more heteroatoms, (vi) and their mixts., such that when the auxiliary is one or more unsatd. hydrocarbon, then this is combined with at least one other auxiliary of a different type. Preferably, $\text{ClSiMe}_2(\text{CH}_2)_3\text{Cl}$ is prepared from ClMe_2SiH and allyl chloride in presence of $[\text{Ir}(\text{COD})\text{Cl}]_2$ and an auxiliary as defined above. In an example, treating 1.194 mol allyl chloride with 1.117 mol ClMe_2SiH in presence of 2.829×10^{-5} mol $[\text{Ir}(\text{COD})\text{Cl}]_2$, 10.9 mmol cyclohexanone and 5.648 mmol COD for 2h 30 min at 20-25° and subsequent stirring for 20 min gave 98.3% $\text{ClSiMe}_2(\text{CH}_2)_3\text{Cl}$.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 1 A + B ==> C





C
YIELD 98%

RX(1) RCT A 1066-35-9, B 107-05-1
PRO C 10605-40-0
CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 108-94-1 Cyclohexanone, 111-78-4 1,5-COD
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 2.5 hours, 20 - 25 deg C
SUBSTAGE(3) 20 minutes, room temperature

L64 ANSWER 3 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 139:22334 CASREACT
TITLE: Method for obtaining bis(monoorganoxysilylpropyl) polysulfides
INVENTOR(S): Guennouni, Nathalie; Pevere, Virginie; Vogin, Bernard
PATENT ASSIGNEE(S): Rhodia Chimie, Fr.
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003048169	A1	20030612	WO 2002-FR4204	20021206
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
FR 2833264	A1	20030613	FR 2001-15768	20011206
FR 2833264	B1	20050819		
FR 2833265	A1	20030613	FR 2002-10145	20020809
FR 2833265	B1	20060210		
AU 2002364429	A1	20030617	AU 2002-364429	20021206
EP 1461344	A1	20040929	EP 2002-799785	20021206
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2005511700	T2	20050428	JP 2003-549359	20021206
EP 1621543	A1	20060201	EP 2005-21616	20021206
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PRIORITY APPLN. INFO.:			FR 2001-15768	20011206
			FR 2002-10145	20020809

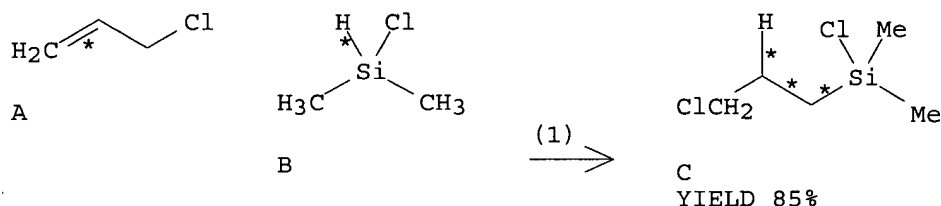
EP 2002-799785 20021206
WO 2002-FR4204 20021206

OTHER SOURCE(S): MARPAT 139:22334

AB The invention concerns the preparation of bis(monoorganooxysilylpropyl) polysulfides $R_1OSiR_2R_3(CH_2)_3-S_x-(CH_2)_3SiR_2R_3OR_1$ (I, $R_1 = C_1-C_{15}$ alkyl, alkoxyalkyl; R_2 and $R_3 = C_1-C_6$ alkyl and/or phenyl; $1.5 \pm 0.1 \leq x \leq 5 \pm 0.1$). Said preparation is carried out by performing successively the following steps (a), (b) and (c): (a) hydrosilylation of the type: $R_2R_3HSi-Hal + CH_2:CH-CH_2-Hal \rightarrow Hal-R_2R_3Si-(CH_2)_3Hal$; (b) alcoholysis of the type: $Hal-R_2R_3Si-(CH_2)_3-Hal + R_1OH \rightarrow R_1O-R_2R_3Si-(CH_2)_3Hal$; (c) sulfidization of the type: $R_1O-R_2R_3Si-(CH_2)_3Hal + M_2S_x \rightarrow$ compound I; with $Hal =$ halogen atom and $M =$ alkali metal. Variations of the above reaction are also included in the invention. Thus, reaction of Me_2HSiCl with $CH_2:CHCH_2Cl$ in the presence of $[Ir(COD)Cl]_2$ ($COD = 1,5$ -cyclooctadiene) as catalyst afforded $ClSiMe_2(CH_2)_3Cl$ (85% yield), which reacted with ethanol to give $EtOSiMe_2(CH_2)_3Cl$ (96% yield). Finally, reaction of the latter with Na_2S_4 afforded bis(monoorganooxysilylpropyl) tetrasulfide, $EtOSiMe_2(CH_2)_3-S_4-(CH_2)_3SiMe_2OEt$ (87% yield).

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 6 A + B ==> C...



RX(1) RCT A 107-05-1

STAGE(1)

CAT **12112-67-3** Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-
CON 20 deg C

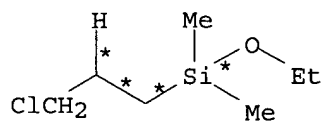
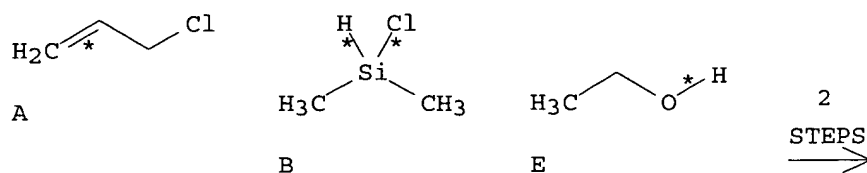
STAGE(2)

RCT B **1066-35-9**
CON SUBSTAGE(1) 155 minutes, 20 - 25 deg C
SUBSTAGE(2) 20 minutes, 20 - 25 deg C

PRO C **10605-40-0**
NTE key step

RX(4) OF 6 COMPOSED OF RX(1), RX(2)

RX(4) A + B + E ==> F



YIELD 96%

RX(1) RCT A 107-05-1

STAGE(1)

CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-
η)-1,5-cyclooctadiene]di-
CON 20 deg C

STAGE(2)

RCT **B 1066-35-9**
CON SUBSTAGE(1) 155 minutes, 20 - 25 deg C
 SUBSTAGE(2) 20 minutes, 20 - 25 deg C

PRO C 10605-40-0
NTE key step

RX(2) RCT C 10605-40-0

STAGE(1)

CON 150 deg C, 1 atm

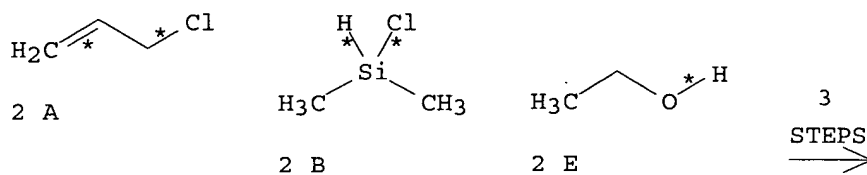
STAGE(2)

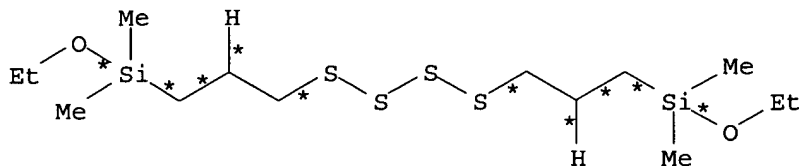
RCT **E 64-17-5**
CON 4.5 hours, 110 deg C, 1 atm

PRO **F 13508-63-9**

RX(6) OF 6 COMPOSED OF RX(1), RX(2), RX(3)

RX(6) 2 A + 2 B + 2 E ==> G





G
YIELD 87%

RX(1) RCT A 107-05-1

STAGE(1)

CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-
CON 20 deg C

STAGE(2)

RCT B 1066-35-9
CON SUBSTAGE(1) 155 minutes, 20 - 25 deg C
SUBSTAGE(2) 20 minutes, 20 - 25 deg C

PRO C 10605-40-0
NTE key step

RX(2) RCT C 10605-40-0

STAGE(1)

CON 150 deg C, 1 atm

STAGE(2)

RCT E 64-17-5
CON 4.5 hours, 110 deg C, 1 atm

PRO F 13508-63-9

RX(3)

STAGE(1)

RGT H 12034-39-8 Sodium sulfide (Na₂(S₄))
SOL 64-17-5 EtOH
CON 80 deg C

STAGE(2)

RCT F 13508-63-9
CON SUBSTAGE(1) 80 deg C
SUBSTAGE(2) 2 hours, 80 deg C

PRO G 298689-48-2

L64 ANSWER 4 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 4

ACCESSION NUMBER: 138:287818 CASREACT

TITLE: Method for preparation of carboxylic acid
3-(dimethylchlorosilyl)propyl ester by hydrosilylation
of carboxylic acid allyl ester with
dimethylchlorosilane

INVENTOR(S): Nishiwaki, Hiromi; Kiyomori, Ayumu; Kubota, Toru;

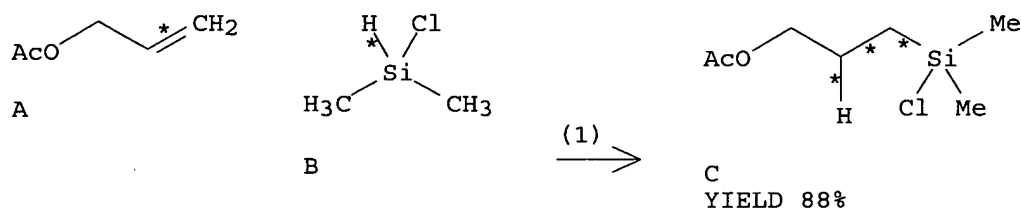
PATENT ASSIGNEE(S): Tonomura, Yoichi
 SOURCE: Shin-Etsu Chemical Industry Co., Ltd., Japan
 Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003096086	A2	20030403	JP 2001-296148	20010927
PRIORITY APPLN. INFO.:			JP 2001-296148	20010927

OTHER SOURCE(S): MARPAT 138:287818

AB Carboxylic acid 3-(dimethylchlorosilyl)propyl esters represented by general formula $\text{RCO}_2(\text{CH}_2)_3\text{SiMe}_3\text{Cl}$ (R = C1-10 monovalent hydrocarbon group) are prepared by hydrosilylation of a carboxylic acid allyl ester of formula $\text{RCO}_2\text{CH}_2\text{CH}=\text{CH}_2$ (R = same as above) with dimethylchlorosilane in the presence of an iridium catalyst. The iridium catalyst is an iridium salt or an iridium complex represented by a general formula $[\text{Ir}(\text{R}_5)\text{Y}]_3$ (R_5 = diene compound; Y = Cl, Br, iodo) and the hydrosilylation is carried out also in the presence of an ethylene derivative of formula $\text{R}_1\text{R}_3\text{C}=\text{CR}_2\text{R}_4$ (wherein R_1 , R_2 = C1-10 monovalent hydrocarbon group; or R_1 and R_2 are bonded to each other to form a C3-20 ring together with the carbon atom to which they are bonded; R_3 , R_4 = H, C1-10 monovalent hydrocarbon group). This process sufficiently decreases the side reactions which presented problems in the past and gives in high yields the desired carboxylic acid 3-(dimethylchlorosilyl)propyl esters of high purity. The carboxylic acid 3-(dimethylchlorosilyl)propyl esters are widely used in industries as silane coupling agents, raw materials for modified silicon oils, and polymerizable monomers for silicon-containing polymers. Thus, allyl methacrylate 26.0, 2,6-di-tert-butyl-4-methylphenol (BHT) (polymerization inhibitor) 0.33, 1,5-cyclooctadiene 2.2, and di- μ -chlorobis(μ -1,5-cyclooctadiene)diiridium 0.017 g were added to a 4-neck 500 mL-flask equipped with a dropping funnel, a Dimroth condenser, a stirrer, and a thermometer and heated to 60° while passing N through an inlet of the condenser, followed by feeding dropwise 94.6 g dimethylchlorosilane over 5.5 h while maintaining the reaction temperature at 60-65° by adjusting the dropping rate or through a heat medium, and the resulting mixture was aged at 60° for 0.4 5 h, cooled to room temperature to give 84.2% 3-(dimethylchlorosilyl)propyl methacrylate (I), 0.2% β -addition isomers, 0.2 methacryloxydimethylsilane, and 0.8% dimethyldichlorosilane as compared to 69.9% I, 2.4% β -adduct, 4.1% methacryloxydimethylsilane, and 2.4% dimethyldichlorosilane when chloroplatinic acid was used as the catalyst. The reaction mixture was distilled by a simple distillation apparatus to first distill volatile components at 38-48° (column top. temperature) and 2.4 KPa and then obtain 179.9 g of the main fraction containing 98.8% I and 0.2% β -adduct at 0.5 kPa (81.5 yield of I) and 48-85° (column top. temperature). Similarly, 3-(dimethylchlorosilyl)propyl acetate was obtained in 87.5% yield from allyl acetate and dimethyldichlorosilane.

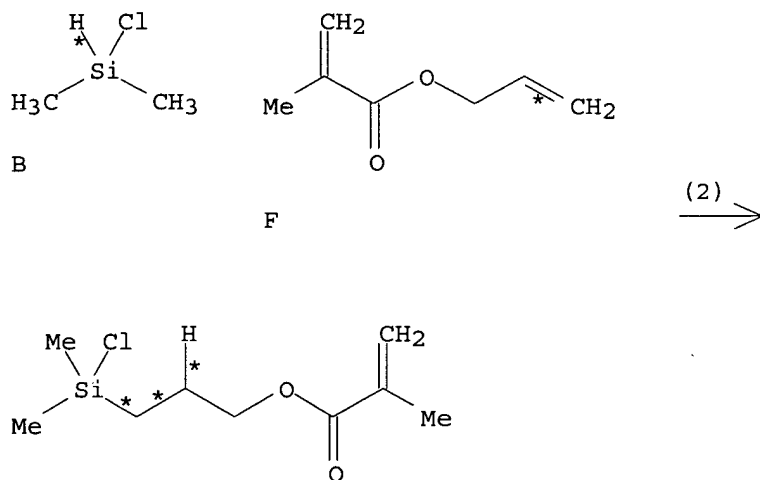
RX(1) OF 2 A + B ==> C



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RX(1)      RCT  A 591-87-7, B 1066-35-9
           PRO  C 18387-98-9
           CAT  12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-
           1,5-cyclooctadiene]di-, 111-78-4 1,5-COD
           CON  SUBSTAGE(1) 4 hours, 75 - 80 deg C
           SUBSTAGE(2) 1 hour, 80 deg C
           NTE  hydrosilylation

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$$\text{RX (2)} \quad \text{OF 2} \quad \mathbf{B} + \mathbf{F} \implies \mathbf{G}$$


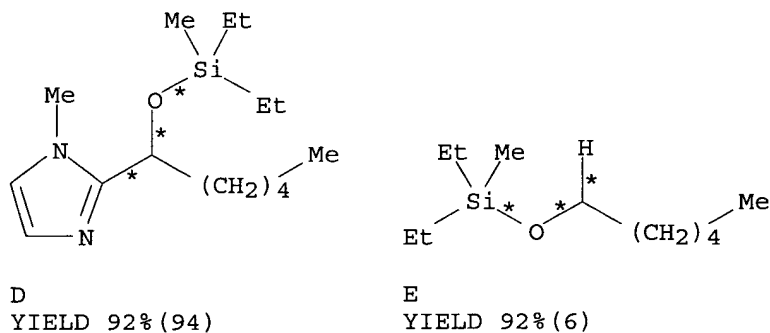
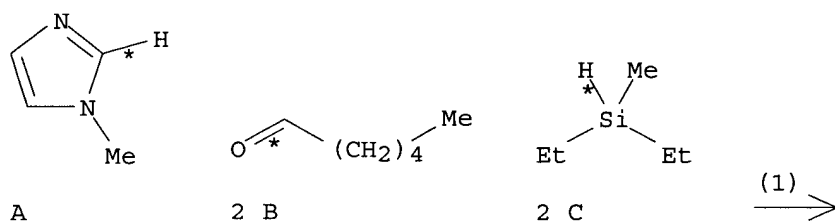
G
YIELD 84%

RX(2) RCT B 1066-35-9, F 96-05-9
PRO G 24636-31-5
CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-
1,5-cyclooctadiene]di-, 111-78-4 1,5-COD
CON SUBSTAGE(1) 5.5 hours, 60 - 65 deg C
SUBSTAGE(2) 0.5 hours, 60 deg C
NTE hydrosilylation

L64 ANSWER 5 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 138:55912 CASREACT
TITLE: [Ir₄(CO)₁₂]-catalyzed coupling reaction of imidazoles
with aldehydes in the presence of a hydrosilane to
give 2-substituted imidazoles

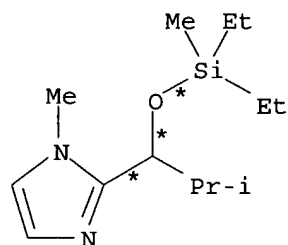
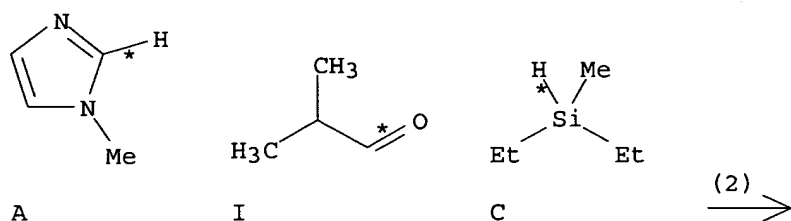
AUTHOR(S): Fukumoto, Yoshiya; Sawada, Katsutoshi; Hagihara, Motoyuki; Chatani, Naoto; Murai, Shinji
 CORPORATE SOURCE: Department of Applied Chemistry Faculty of Engineering, Osaka University, Osaka, 565-0871, Japan
 SOURCE: Angewandte Chemie, International Edition (2002), 41(15), 2779-2781
 CODEN: ACIEF5; ISSN: 1433-7851
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A significant increase in yield is observed when DMAD is added to the reaction of 1-methylimidazole with aldehydes and diethylmethylsilane in the presence of a catalytic amount of [Ir₄(CO)₁₂] to produce 2-(1-diethylmethylsiloxyalkyl)imidazoles.
 REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 10 A + 2 B + 2 C ==> D + E



RX(1) RCT A 616-47-7, B 66-25-1, C 760-32-7
 PRO D 479496-25-8, E 479496-26-9
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro,
 762-42-5 DMADC
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> reflux
 SUBSTAGE(3) 2 hours, reflux
 SUBSTAGE(4) reflux -> room temperature

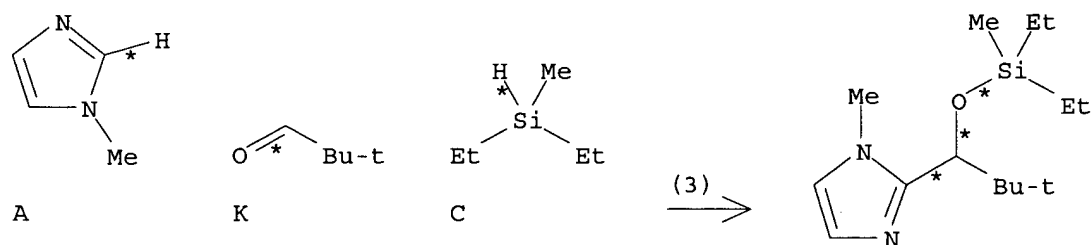
RX(2) OF 10 A + I + C ==> J



J
YIELD 91%

RX(2) RCT A 616-47-7, I 78-84-2, C 760-32-7
 PRO J 479496-27-0
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro,
 762-42-5 DMADC
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> reflux
 SUBSTAGE(3) 3 hours, reflux
 SUBSTAGE(4) reflux -> room temperature

RX(3) OF 10 A + K + C ==> L

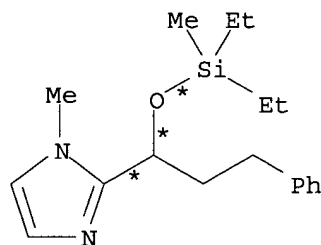
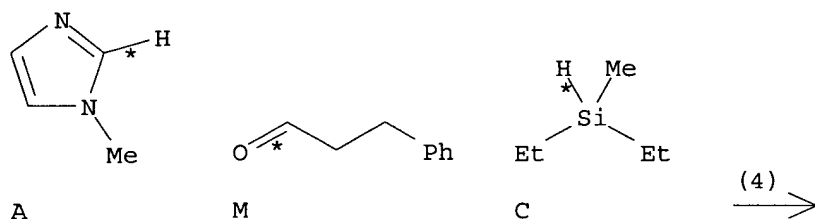


L
YIELD 76%

RX(3) RCT A 616-47-7, K 630-19-3, C 760-32-7
 PRO L 479496-28-1
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro,

762-42-5 DMADC
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> reflux
 SUBSTAGE(3) 4 hours, reflux
 SUBSTAGE(4) reflux -> room temperature

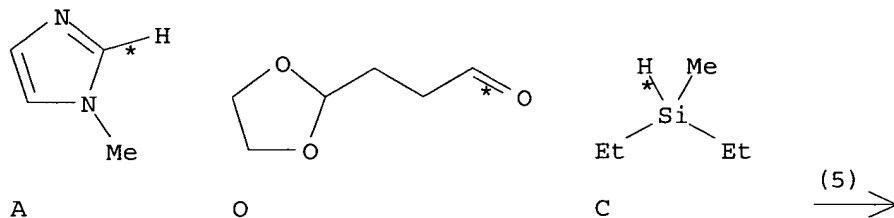
RX(4) OF 10 A + M + C ==> N

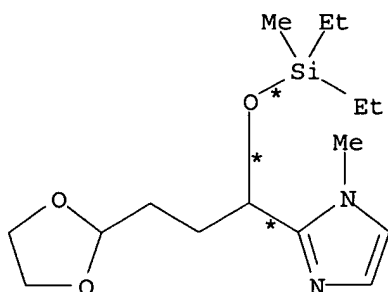


N
 YIELD 72%

RX(4) RCT A 616-47-7, M 104-53-0, C 760-32-7
 PRO N 479496-29-2
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro,
 762-42-5 DMADC
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> reflux
 SUBSTAGE(3) 1 hour, reflux
 SUBSTAGE(4) reflux -> room temperature

RX(5) OF 10 A + O + C ==> P

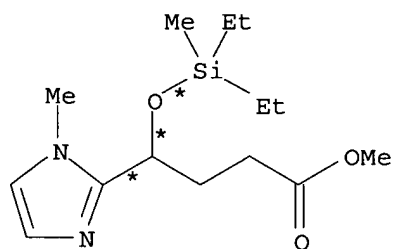
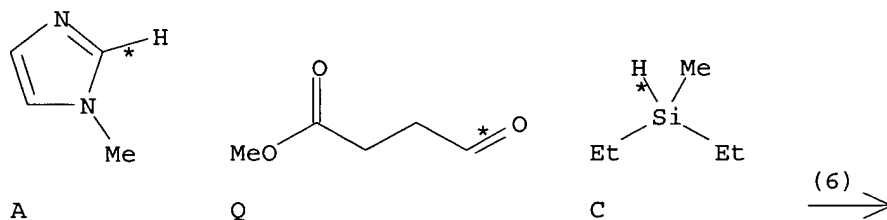




P
YIELD 62%

RX(5) RCT A 616-47-7, O 82962-18-3, C 760-32-7
 PRO P 479496-30-5
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro,
 762-42-5 DMADC
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> reflux
 SUBSTAGE(3) 1 hour, reflux
 SUBSTAGE(4) reflux -> room temperature

RX(6) OF 10 A + Q + C ==> R

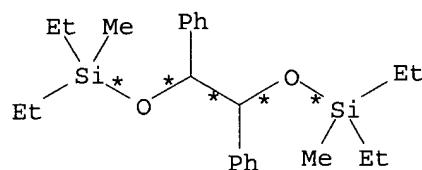
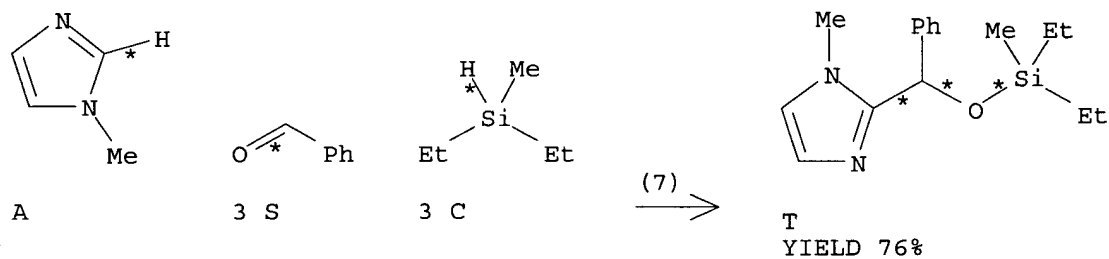


R
YIELD 87%

RX(6) RCT A 616-47-7, Q 13865-19-5, C 760-32-7
 PRO R 479496-31-6
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro,

762-42-5 DMADC
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> reflux
 SUBSTAGE(3) 1 hour, reflux
 SUBSTAGE(4) reflux -> room temperature

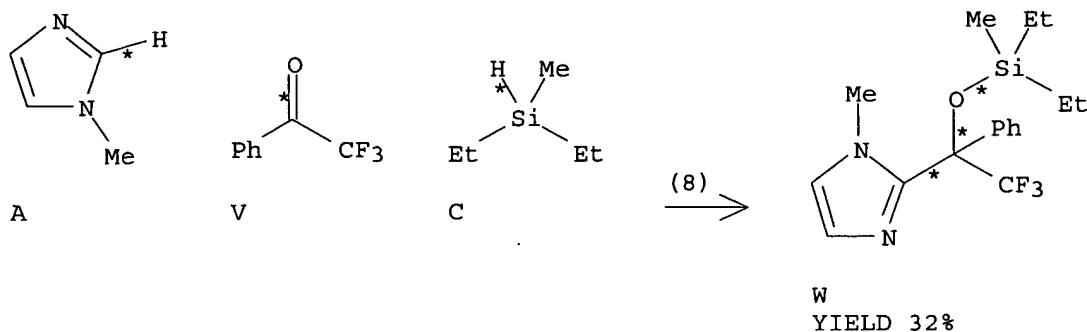
RX(7) OF 10 A + 3 S + 3 C ==> T + U



U
YIELD 8%

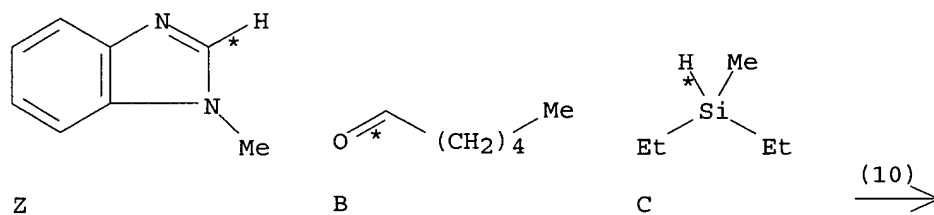
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 PRO T 479496-32-7, U 96206-22-3
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro,
 762-42-5 DMADC
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> reflux
 SUBSTAGE(3) 2 hours, reflux
 SUBSTAGE(4) reflux -> room temperature

RX(8) OF 10 A + V + C ==> W



RX(8) RCT A 616-47-7, V 434-45-7, C 760-32-7
 PRO W 479496-33-8
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro,
 762-42-5 DMADC
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> reflux
 SUBSTAGE(3) 3 hours, reflux
 SUBSTAGE(4) reflux -> room temperature

RX(10) OF 10 Z + B + C ==> AA



RX(10) RCT Z 1632-83-3, B 66-25-1, C 760-32-7
 PRO AA 479496-35-0
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro,
 762-42-5 DMADC

SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> reflux
 SUBSTAGE(3) 19 hours, reflux
 SUBSTAGE(4) reflux -> room temperature

L64 ANSWER 6 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 6
 ACCESSION NUMBER: 135:371860 CASREACT
 TITLE: Preparation of halopropyltrimethylchlorosilanes
 INVENTOR(S): Tonomura, Yoichi; Kubota, Toru; Endo, Mikio
 PATENT ASSIGNEE(S): Shin-Etsu Chemical Industry Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001322993	A2	20011120	JP 2000-142128	20000515
US 2001053861	A1	20011220	US 2001-852638	20010511
US 6359161	B2	20020319		
EP 1156052	A2	20011121	EP 2001-304327	20010515
EP 1156052	A3	20030917		
EP 1156052	B1	20060208		

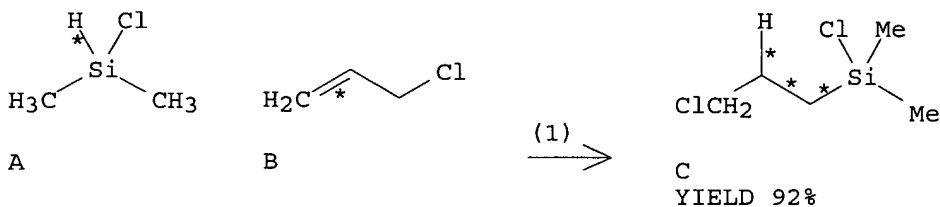
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

PRIORITY APPLN. INFO.: JP 2000-142128 20000515

OTHER SOURCE(S): MARPAT 135:371860

AB The compds. XCH₂CH₂CH₂SiMe₂Cl (X = Cl, Br, I) are prepd by reaction of Me₂SiHCl with XCH₂CH:CH₂ (X = same as above) in the presence of Ir catalysts and R₁CR₃C:CR₂R₄ (R₁, R₂ = C₁-10 hydrocarbyl; R₁R₂ may form ring; R₃, R₄ = H, C₁-10 hydrocarbyl). Me₂SiHCl was reacted with allyl chloride in the presence of di-μ-chlorobis(μ-1,5-cyclooctadiene)diiridium and 1,5-cyclooctadiene at 35-40° for 7 h to give 92.7% 3-chloropropyltrimethylchlorosilane.

RX(1) OF 1 A + B ==> C



RX(1) RCT A 1066-35-9, B 107-05-1
 PRO C 10605-40-0
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 111-78-4 1,5-COD

L64 ANSWER 7 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 7
 ACCESSION NUMBER: 131:116373 CASREACT

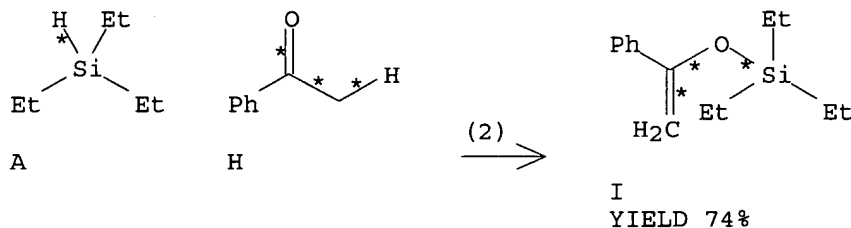
TITLE: Preparation of silyl enol ethers
 INVENTOR(S): Fuchigami, Takamasa; Igarashi, Yasushi
 PATENT ASSIGNEE(S): Sagami Chemical Research Center, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11217391	A2	19990810	JP 1998-15904	19980128
PRIORITY APPLN. INFO.:			JP 1998-15904	19980128

OTHER SOURCE(S): MARPAT 131:116373

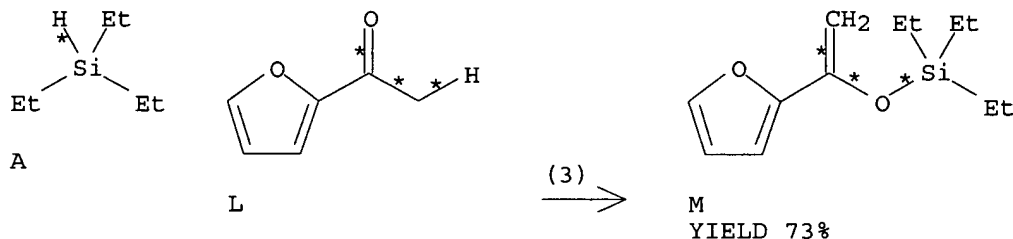
AB Title compds. RC(OSiR₁R₂R₃):CR₄R₅ (R, R₁, R₂, R₃, R₄, R₅ = H, alkyl, aryl, etc.) were prepared by reaction of ketones RCOCHR₄R₅ with HSiR₁R₂R₃ in the presence of group 7-10 metals, halides, and amines. Thus, reaction of cyclohexanone with Et₃SiH in toluene in the presence of 5% Pd/C, EtI, and Et₃N at 100° for 16 h gave 87.1% 1-triethylsiloxy-cyclohexene.

RX(2) OF 3 A + H ==> I



RX(2) RCT A 617-86-7, H 98-86-2
 PRO I 17718-70-6
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro,
 75-03-6 EtI, 109-89-7 Et₂NH
 SOL 108-88-3 PhMe

RX(3) OF 3 A + L ==> M



RX(3) RCT A 617-86-7, L 1192-62-7
 PRO M 220800-79-3

CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro,
75-03-6 EtI, 109-89-7 Et₂NH
SOL 108-88-3 PhMe

L64 ANSWER 8 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 8

ACCESSION NUMBER: 130:196694 CASREACT

TITLE: Transition metal-catalyzed dehydrogenative silylation
of ketones with amine and halide as cocatalysts

AUTHOR(S): Igarashi, Mamoru; Sugihara, Yuichi; Fuchikami,
Takamasa

CORPORATE SOURCE: Sagami Chemical Research Center, Kanagawa, 229-0012,
Japan

SOURCE: Tetrahedron Letters (1999), 40(4), 711-714

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

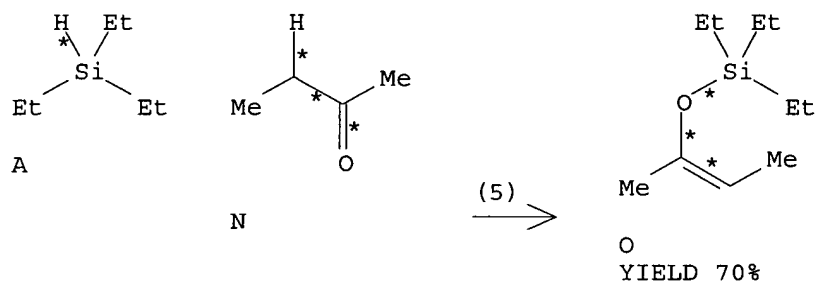
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Dehydrogenative silylation of ketones with hydrosilanes proceeds in the
presence of a transition metal catalyst such as Pd on C or Ir carbonyl,
with amine and halide as cocatalysts, to give the corresponding silyl enol
ethers in good yields. The present reaction is applicable for a variety
of ketones and hydrosilanes with complete regioselectivity.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(5) OF 11 A + N ==> O



RX(5) RCT A **617-86-7**, N 78-93-3

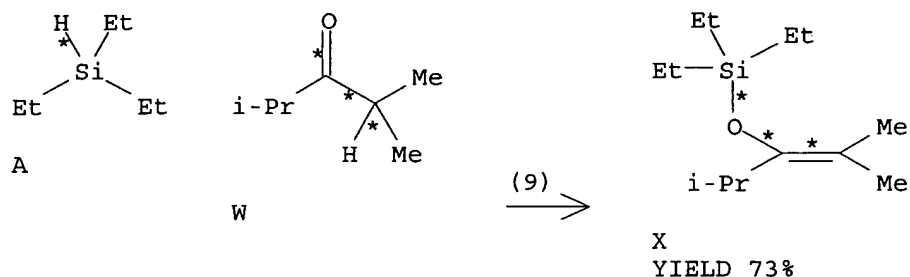
PRO O **13829-50-0**

CAT 109-89-7 Et₂NH, 75-03-6 EtI, **18827-81-1** Iridium,
dodecacarbonyltetra-, tetrahedro

SOL 108-88-3 PhMe

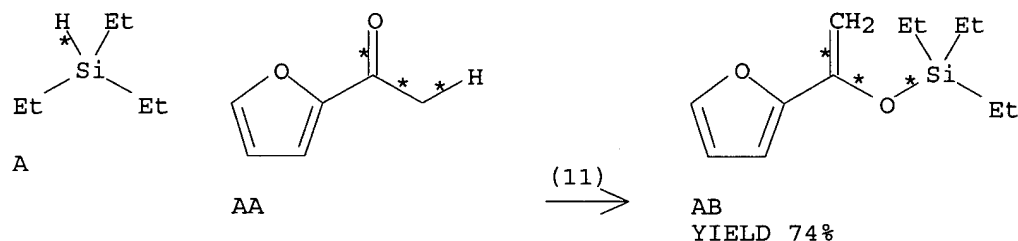
NTE regioselective

RX(9) OF 11 A + W ==> X



RX(9) RCT A 617-86-7, W 565-80-0
 PRO X 80239-20-9
 CAT 109-89-7 Et₂NH, 75-03-6 EtI, 18827-81-1 Iridium,
 dodecacarbonyltetra-, tetrahedro
 SOL 108-88-3 PhMe
 NTE regioselective

RX(11) OF 11 A + AA ==> AB



RX(11) RCT A 617-86-7, AA 1192-62-7
 PRO AB 220800-79-3
 CAT 109-89-7 Et₂NH, 75-03-6 EtI, 18827-81-1 Iridium,
 dodecacarbonyltetra-, tetrahedro
 SOL 108-88-3 PhMe
 NTE regioselective

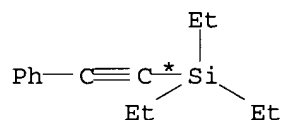
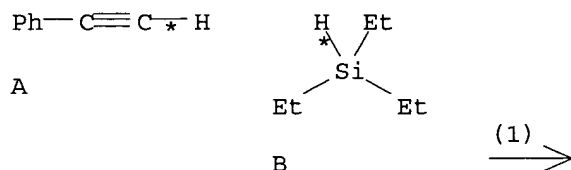
L64 ANSWER 9 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 9
 ACCESSION NUMBER: 127:358956 CASREACT
 TITLE: Process for preparation of alkynylsilanes by
 catalytic coupling reaction
 INVENTOR(S): Fuchigami, Takamasa; Shimizu, Rie
 PATENT ASSIGNEE(S): Zaidan Hojin Sagami Chemical Research Center, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 09295986 A2 19971118 JP 1996-340782 19961220
 PRIORITY APPLN. INFO.: JP 1996-51350 19960308
 OTHER SOURCE(S): MARPAT 127:358956

AB The title compds. R'C.tplbond.CSiR₃ (I; R = alkyl, alkenyl, aryl, etc.; R' = H, alkyl, alkenyl, aryl, etc.), are prepared by reacting HSiR₃ with R'C.tplbond.CH (II; R' = same as above) in the presence of iridium carbonyl catalysts. I, useful materials in organic synthesis, are prepared in high yield easily. Thus, II (R' = Ph) was reacted with HSiEt₃ in the presence of Ir₄(CO)₁₂ at 100° for 24 h to give 96% I (R = Et, R' = Ph).

RX(1) OF 1 A + B ==> C



C
YIELD 96%

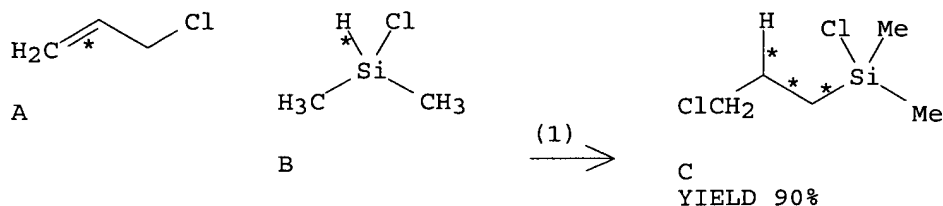
RX(1) RCT A 536-74-3, B 617-86-7
 PRO C 4131-43-5
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro,
 603-35-0 PPh₃
 SOL 110-71-4 (CH₂OMe)₂
 NTE 100° for 24 h

L64 ANSWER 10 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 10
 ACCESSION NUMBER: 123:340390 CASREACT
 TITLE: Preparation of (halopropyl)dimethylchlorosilane and
 catalysts used in the preparation
 INVENTOR(S): Kubota, Tooru; Yamamoto, Akira; Endo, Mikio
 PATENT ASSIGNEE(S): Shinetsu Chemical Industry Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07126271	A2	19950516	JP 1993-270278	19931028
JP 2938731	B2	19990825		
PRIORITY APPLN. INFO.:			JP 1993-270278	19931028
OTHER SOURCE(S):		MARPAT 123:340390		

AB (Halopropyl)dimethylchlorosilane, useful as an intermediate for silane coupling agents and as a modifier for silicone oils (no data), is prepared by treatment of Me_2SiHCl with $\text{XCH}_2\text{CH}:\text{CH}_2$ ($\text{X} = \text{Cl}, \text{Br}, \text{I}$) in the presence of $[\text{IrRY}]_2$ ($\text{R} = \text{diene}; \text{Y} = \text{Cl}, \text{Br}, \text{I}$). Me_2SiHCl was added dropwise to a mixture of allyl chloride and di- μ -chlorobis(η^4 -1,5-cyclooctadiene)diiridium at 35-40° over 1 h and left at 40° for 1 h to give 90.5% (3-chloropropyl)dimethylchlorosilane.

RX(1) OF 1 A + B ==> C

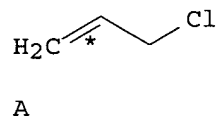


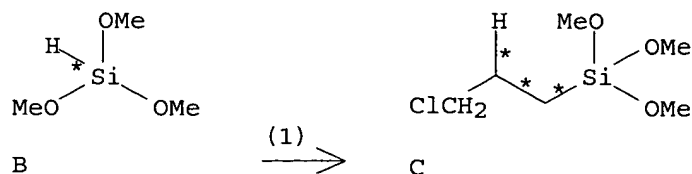
RX(1) RCT A 107-05-1, B 1066-35-9
 PRO C 10605-40-0
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-

L64 ANSWER 11 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 11
 ACCESSION NUMBER: 119:180892 CASREACT
 TITLE: Ruthenium complex-catalyzed hydrosilylation of allyl chloride with trimethoxysilane
 AUTHOR(S): Tanaka, Masato; Hayashi, Teruyuki; Mi, Zhi Yuan
 CORPORATE SOURCE: Natl. Chem. Lab. Ind., Tsukuba, 305, Japan
 SOURCE: Journal of Molecular Catalysis (1993), 81(2), 207-14
 CODEN: JMCADS; ISSN: 0304-5102
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The hydrosilylation of allyl chloride with trimethoxysilane has been examined in the presence of several homogeneous complex catalysts. Iridium and ruthenium complexes exhibit higher selectivities in the reaction to give (3-chloropropyl)trimethoxysilane. Other complexes usually give propylene and/or tetramethoxysilane as side products in large quantities. The $\text{Ru}_3(\text{CO})_{12}$ -catalyzed reactions effected at lower temps. or by using a large excess of trimethoxysilane relative to allyl chloride give the chloropropylsilane in good yields.

RX(1) OF 2 A + B ==> C

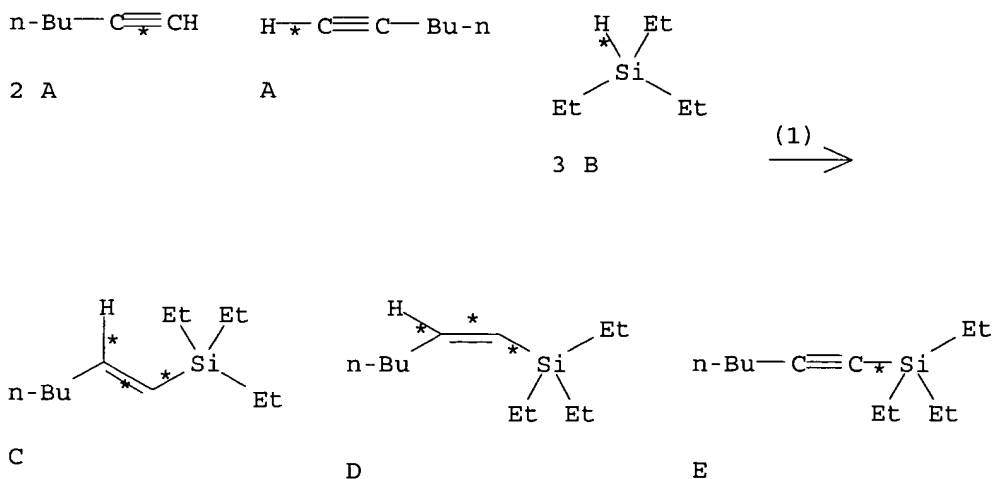




RX(1) RCT A 107-05-1, B **2487-90-3**
 PRO C **2530-87-2**
 CAT **12246-51-4** Cyclooctene Ir
 SOL 108-88-3 PhMe
 NTE other products also formed

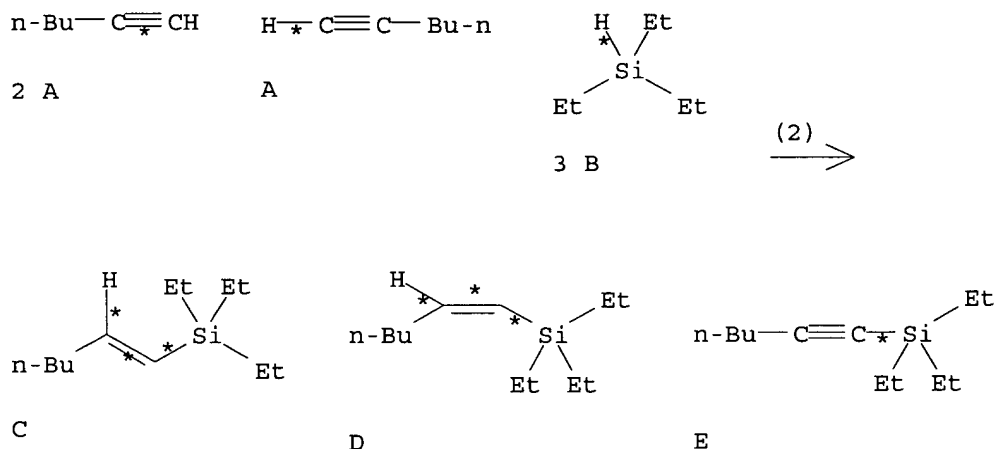
L64 ANSWER 12 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 12
 ACCESSION NUMBER: 110:24071 CASREACT
 TITLE: Iridium catalyzed hydrosilylation of 1-hexyne: the unusual formation of 1-(triethylsilyl)-1-hexyne
 AUTHOR(S): Fernandez, Maria J.; Oro, Luis A.; Manzano, Blanca R.
 CORPORATE SOURCE: Inst. Cienc. Mater. Aragon, Univ. Zaragoza, Zaragoza, 50009, Spain
 SOURCE: Journal of Molecular Catalysis (1988), 45(1), 7-15
 CODEN: JMCADS; ISSN: 0304-5102
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 1-Hexyne undergoes reaction with Et₃SiH in the presence of IrH₂(SiEt₃)(COD)(AsPh₃) (COD = 1,5-cyclooctadiene) or Ir catalysts formed by adding triarylsilanes or triarylphosphines to [Ir(OMe)(diolefin)]₂. The products of the catalytic reaction are the expected trans- and cis-1-triethylsilylhex-1-enes, as well as significant amts. of 1-triethylsilylhex-1-yne and 1-hexene. Mechanistic pathways for the observed hydrosilylation reaction are discussed, including the possible participation of a vinylidene-iridium intermediate formed from hydridoalkynyliridium species.

RX(1) OF 7 3 A + 3 B ==> C + D +
 E



RX(1) RCT A 693-02-7, B 617-86-7
 PRO C 42067-72-1, D 62621-38-9, E 21693-13-0
 CAT 94401-81-7 Iridium, di- μ -methoxybis[(2,3,9,10- η)-5,6,7,8-tetrafluoro-1,4-dihydro-1,4-ethenonaphthalene]di-
 SOL 107-06-2 ClCH₂CH₂Cl
 NTE Reaction was also carried out in presence of phosphines or arsines

RX(2) OF 7 3 A + 3 B ==> C + D + E

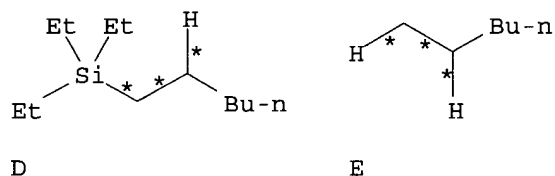
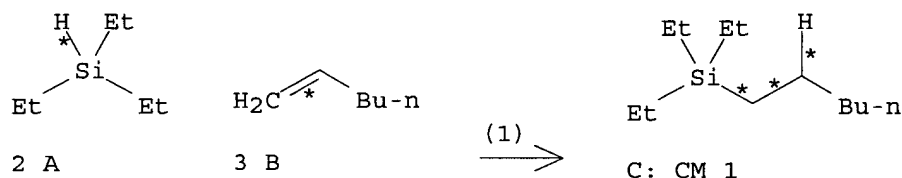


RX(2) RCT A 693-02-7, B 617-86-7
 PRO C 42067-72-1, D 62621-38-9, E 21693-13-0
 CAT 12148-71-9 Iridium, bis[(1,2,5,6- η)-1,5-cyclooctadiene]di- μ -methoxydi-
 SOL 107-06-2 ClCH₂CH₂Cl
 NTE Reaction was also carried out in presence of phosphines or arsines

L64 ANSWER 13 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 13
 ACCESSION NUMBER: 107:59087 CASREACT
 TITLE: Hydrosilylation of alkenes by iridium complexes
 AUTHOR(S): Oro, L. A.; Fernandez, M. J.; Esteruelas, M. A.; Jimenez, M. S.
 CORPORATE SOURCE: Inst. Cienc. Mater. Aragon., Univ. Zaragoza, Saragossa, 50009, Spain
 SOURCE: Journal of Molecular Catalysis (1986), 37(2-3), 151-6
 CODEN: JMCADS; ISSN: 0304-5102
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB [IrX(COD)]₂ (X = OMe, Cl; COD = cyclooctadiene) with monodentate Group Vb atom donor ligands (NPh₃, PPh₃, AsPh₃, SbPh₃) yielded a mixture of hexenyltriethylsilanes as well as the expected hexyltriethylsilane from the catalytic hydrosilylation of hex-1-ene by Et₃SiH. The most effective catalysts are those derived from [IrCl(COD)]₂ + 2 PPh₃ + 2 AsPh₃ and

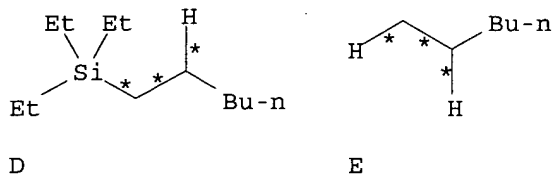
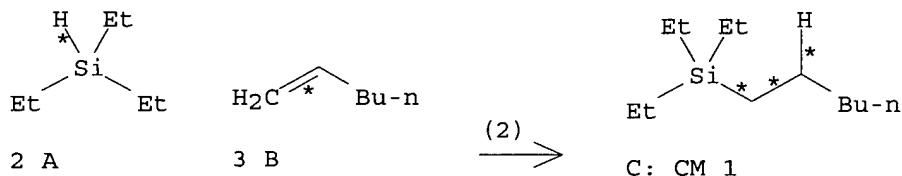
[Ir(OMe)(COD)]₂ + 2 AsPh₃. The latter system was active for hydrosilylation reactions involving ethylene and propylene. The catalyst systems studied include [IrX(COD)]₂ + 2L (X = OMe, L = NPh₃, PPh₃, AsPh₃, SbPh₃; X = Cl, L = PPh₃, AsPh₃), [Ir(OMe)(COD)]₂ + 4L (L = PPh₃, AsPh₃) and [IrX(COD)]₂ + 2PPh₃ + 2AsPh₃ (X = OMe, Cl).

RX(1) OF 14 2 A + 3 B ==> C + D +
E...



RX(1) RCT A 617-86-7, B 592-41-6
 PRO C 109389-69-7, D 13810-04-3, E
 110-54-3
 CAT 12148-71-9 Iridium, bis[(1,2,5,6-η)-1,5-
 cyclooctadiene]di-μ-methoxydi-, 603-34-9 Benzenamine,
 N,N-diphenyl-
 SOL 107-06-2 ClCH₂CH₂Cl

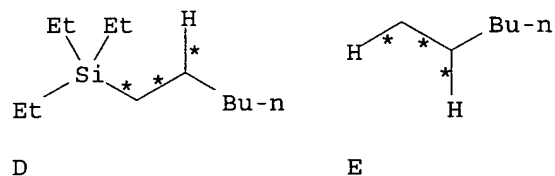
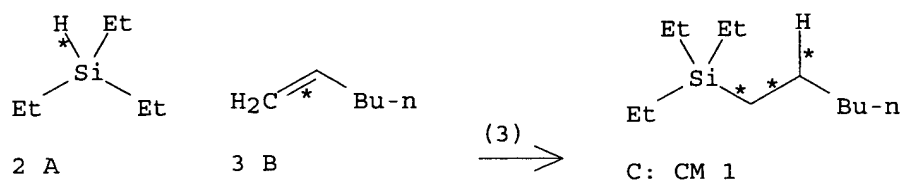
RX(2) OF 14 2 A + 3 B ==> C + D +
E



RX(2) RCT A 617-86-7, B 592-41-6

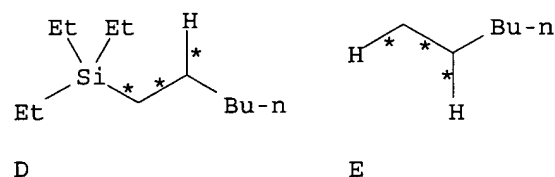
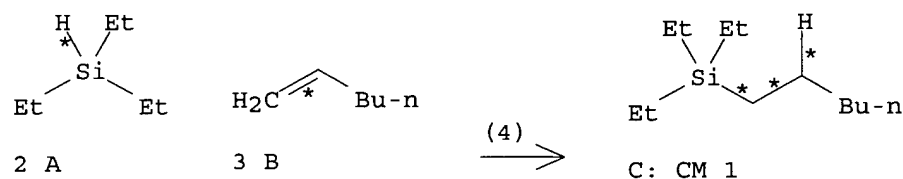
PRO C 109389-69-7, D 13810-04-3, E
 110-54-3
 CAT 12148-71-9 Iridium, bis[(1,2,5,6-η)-1,5-
 cyclooctadiene]di-μ-methoxydi-, 603-35-0 PPh3
 SOL 107-06-2 ClCH2CH2Cl

RX(3) OF 14 2 A + 3 B ==> C + D +
 E



RX(3) RCT A 617-86-7, B 592-41-6
 PRO C 109389-69-7, D 13810-04-3, E
 110-54-3
 CAT 12148-71-9 Iridium, bis[(1,2,5,6-η)-1,5-
 cyclooctadiene]di-μ-methoxydi-, 603-32-7 Ph3As
 SOL 107-06-2 ClCH2CH2Cl

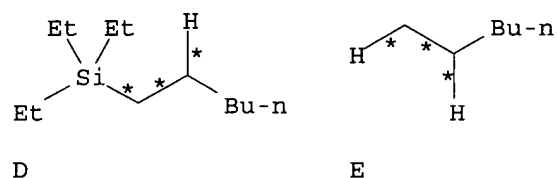
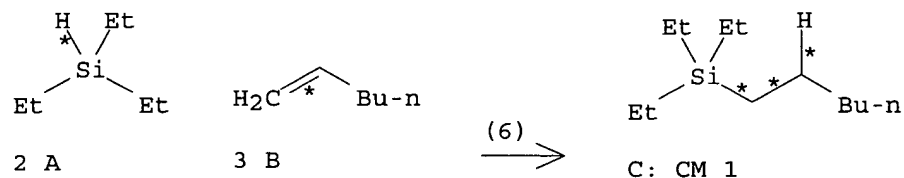
RX(4) OF 14 2 A + 3 B ==> C + D +
 E



RX(4) RCT A 617-86-7, B 592-41-6
 PRO C 109389-69-7, D 13810-04-3, E
 110-54-3

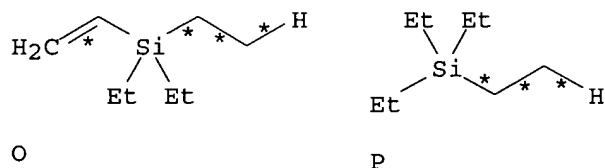
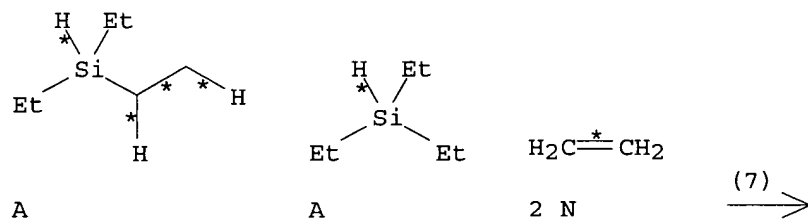
CAT 12148-71-9 Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-, 603-36-1 Ph3Sb
 SOL 107-06-2 ClCH2CH2Cl

RX(6) OF 14 2 A + 3 B ==> C + D +
 E



RX(6) RCT A 617-86-7, B 592-41-6
 PRO C 109389-69-7, D 13810-04-3, E 110-54-3
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 603-32-7 Ph3As
 SOL 107-06-2 ClCH2CH2Cl

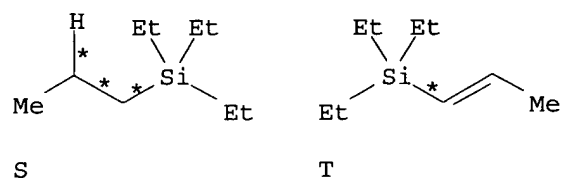
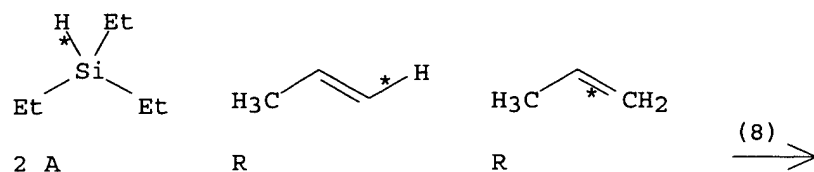
RX(7) OF 14 2 A + 2 N ==> O + P



RX(7) RCT A 617-86-7, N 74-85-1
 PRO O 1112-54-5, P 631-36-7
 CAT 12148-71-9 Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-, 603-32-7 Ph3As

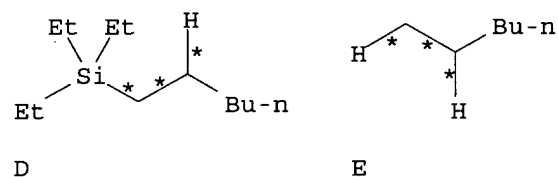
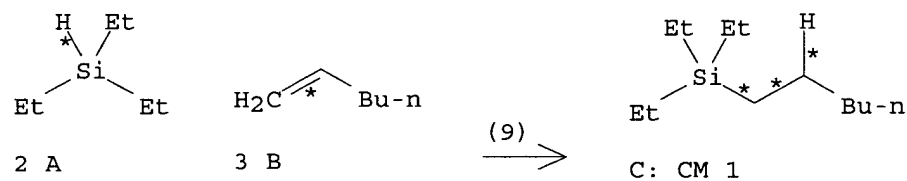
SOL 75-09-2 CH₂Cl₂

RX(8) OF 14 2 A + 2 R ==> S + T



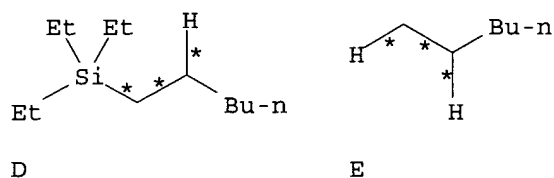
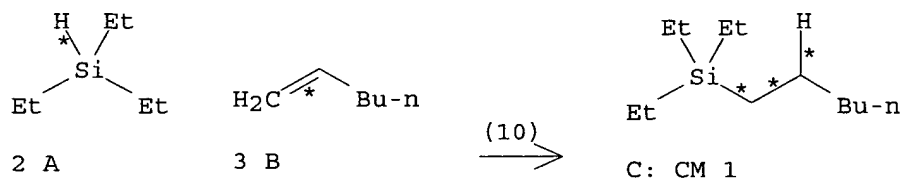
RX(8) RCT A 617-86-7, R 115-07-1
 PRO S 994-44-5, T 3931-84-8
 CAT 12148-71-9 Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-, 603-32-7 Ph₃As
 SOL 75-09-2 CH₂Cl₂

RX(9) OF 14 2 A + 3 B ==> C + D +
 E



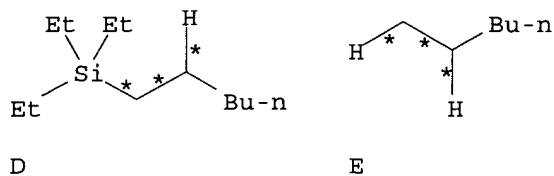
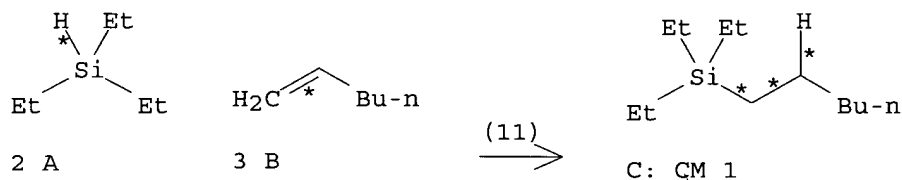
RX(9) RCT A 617-86-7, B 592-41-6
 PRO C 109389-69-7, D 13810-04-3, E 110-54-3
 CAT 12148-71-9 Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-, 603-35-0 PPh₃, 603-32-7 Ph₃As
 SOL 107-06-2 ClCH₂CH₂Cl

RX(10) OF 14 2 A + 3 B ==> C + D +

E

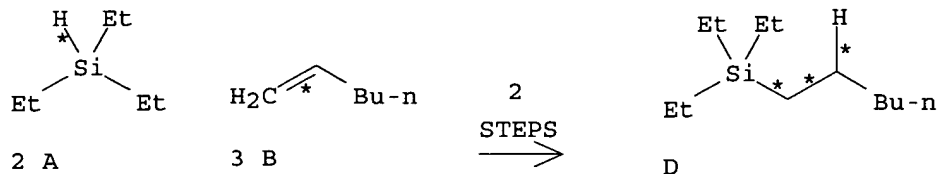
RX(10) RCT A 617-86-7, B 592-41-6
 PRO C 109389-69-7, D 13810-04-3, E
 110-54-3
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-
 1,5-cyclooctadiene]di-, 603-35-0 PPh3, 603-32-7 Ph3As
 SOL 107-06-2 ClCH2CH2Cl

RX(11) OF 14 2 A + 3 B ==> C + D +
 E



RX(11) RCT A 617-86-7, B 592-41-6
 PRO C 109389-69-7, D 13810-04-3, E
 110-54-3
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-
 1,5-cyclooctadiene]di-, 603-35-0 PPh3
 SOL 107-06-2 ClCH2CH2Cl

RX(14) OF 14 COMPOSED OF RX(1), RX(13)
 RX(14) 2 A + 3 B ==> D

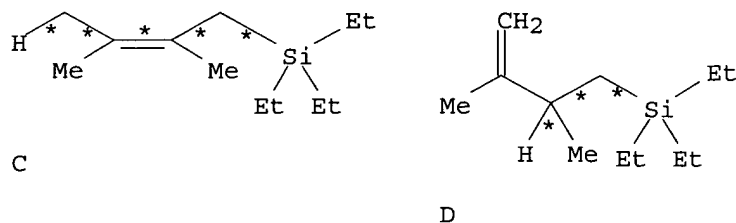
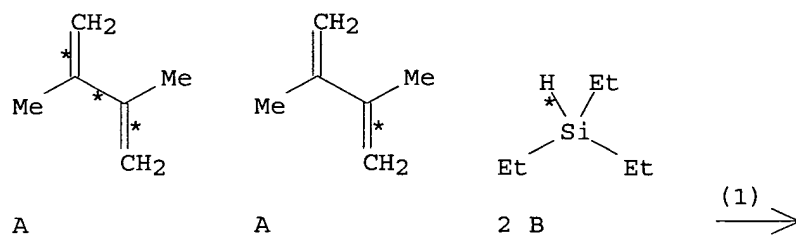


RX(1) RCT A **617-86-7**, B 592-41-6
 PRO C 109389-69-7, D **13810-04-3**, E 110-54-3
 CAT **12148-71-9** Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-, 603-34-9 Benzenamine, N,N-diphenyl-
 SOL 107-06-2 ClCH₂CH₂Cl

RX(13) RCT C 109389-69-7
 RGT Y 1333-74-0 H₂
 PRO D **13810-04-3**
 CAT 52657-94-0 Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, perchlorate

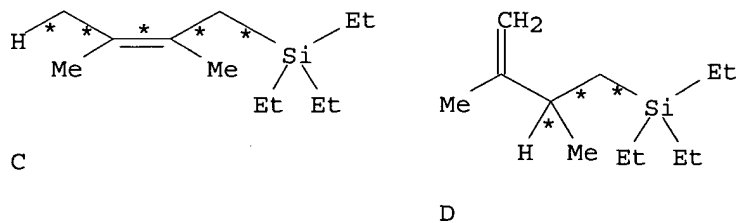
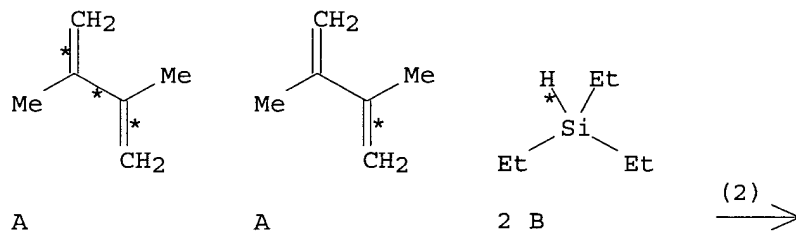
L64 ANSWER 14 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 14
 ACCESSION NUMBER: 103:178404 CASREACT
 TITLE: Iridium complexes as hydrosilylation catalysts
 AUTHOR(S): Apple, David C.; Brady, Karen A.; Chance, Jeffrey M.; Heard, Nina E.; Nile, Terence A.
 CORPORATE SOURCE: Dep. Chem., Univ. North Carolina, Greensboro, NC, 27412, USA
 SOURCE: Journal of Molecular Catalysis (1985), 29(1), 55-64
 CODEN: JMCADS; ISSN: 0304-5102
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB [IrClL₂]₂ (I; L = cyclooctene) (II) catalyzed hydrosilylation of H₂C:CM₂CH₂, giving predominantly the 1,4 adducts Me₂CC:CM₂CH₂SiR₃ (R = Et, OEt); addition of PPh₃ decreased the yield. Hydrosilylation of PrC.tplbond.CH with HSiEt₃ using II or II-PR13 (R₁ = Ph, C₆H₄Me-2) gave 62-100% PrCH:CHSiEt₃ containing 70-83% of the cis isomer. Hydrosilylation of cyclohexanone, in 64-75% yield, was also catalyzed by II or II-PPh₃ but addition of 2 equiv PPh₃ gave the catalytically inert IrHCl(SiEt₃)(PPh₃)₂. Hydrosilylation of 1-octene using II or II-PR13 (same R₁) proceeded in only 4-30% yield to 1-octylsilanes. Hydrosilylation of 2-cyclohexenone with HSiEt₃ using I (L = 1,5-cyclooctadiene) (III) or II occurred largely by 1,2-addition to give 2-cyclohexenol in 69-76% selectively following hydrolysis. Replacing HSiEt₃ with H₂SiMePh gave only 2-cyclohexenol. However, using II-PPh₃ increased the formation of 1,4-addition product in both cases. Attempted asym. induction using MeCOCO₂Et or PhAc, III, H₂SiPh₂, and chiral diphosphines gave 0-7% enantiomeric excesses.

RX(1) OF 43 2 A + 2 B ==> C + D



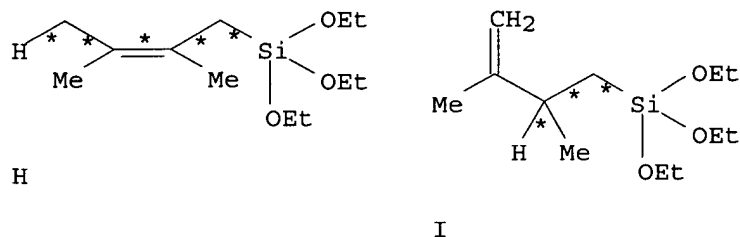
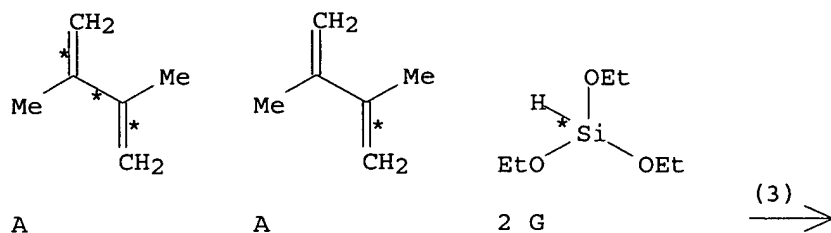
RX(1) RCT A 513-81-5, B 617-86-7
 PRO C 64545-12-6, D 64578-20-7
 CAT 12246-51-4 Cyclooctene Ir
 NTE Reaction was run neat. The 1, 4-adduct was the major product

RX(2) OF 43 2 A + 2 B ==> C + D



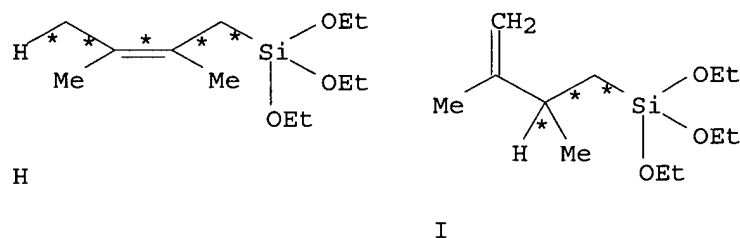
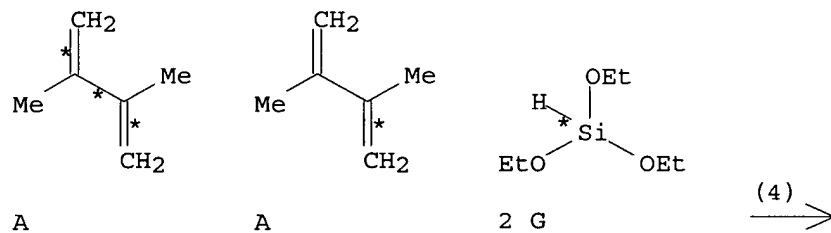
RX(2) RCT A 513-81-5, B 617-86-7
 PRO C 64545-12-6, D 64578-20-7
 CAT 12246-51-4 Cyclooctene Ir, 603-35-0 PPh3
 NTE Reaction was run neat. The 1, 4-adduct was the major product

RX(3) OF 43 2 A + 2 G ==> H + I



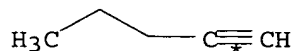
RX(3) RCT A 513-81-5, G 998-30-1
 PRO H 63424-04-4, I 64545-11-5
 CAT 12246-51-4 Cyclooctene Ir
 NTE Reaction was run neat. The 1, 4-adduct was the major product

RX(4) OF 43 2 A + 2 G ==> H + I

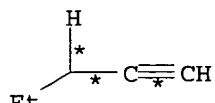


RX(4) RCT A 513-81-5, G 998-30-1
 PRO H 63424-04-4, I 64545-11-5
 CAT 12246-51-4 Cyclooctene Ir, 603-35-0 PPh3
 NTE Reaction was run neat. The 1, 4-adduct was the major product

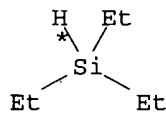
RX(5) OF 43 3 J + 3 B ==> K + L +

M

2 J

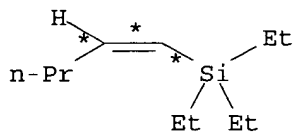


J

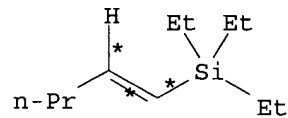


3 B

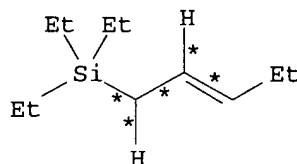
(5) →



K



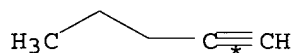
L



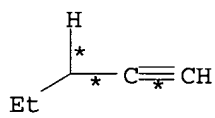
M

RX (5) RCT J 627-19-0, B 617-86-7
 PRO K 68928-08-5, L 68928-07-4, M 40962-02-5
 CAT 12246-51-4 Cyclooctene Ir

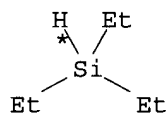
RX (6) OF 43 3 J + 3 B ==> K + L +
M



2 J

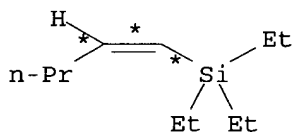


J

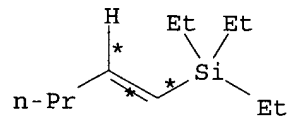


3 B

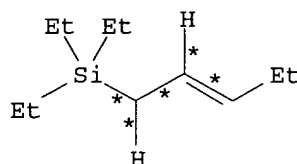
(6) →



K



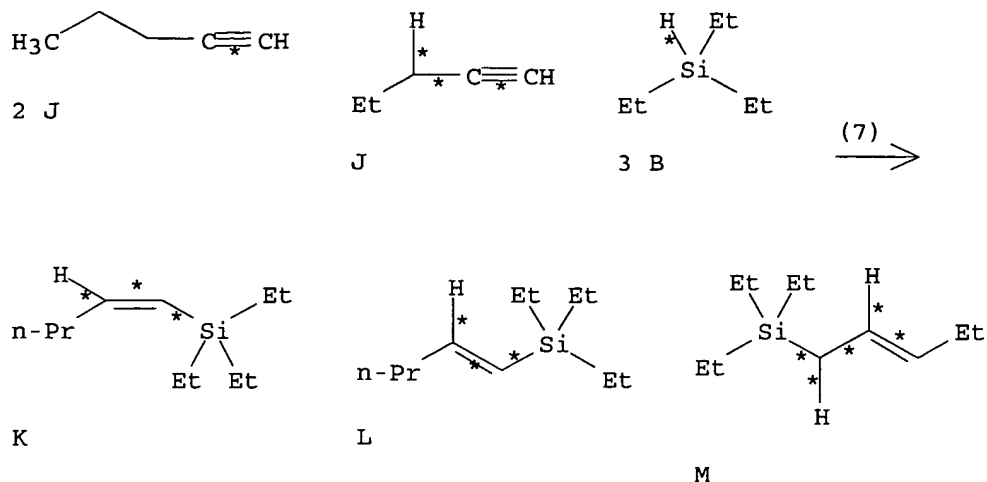
L



M

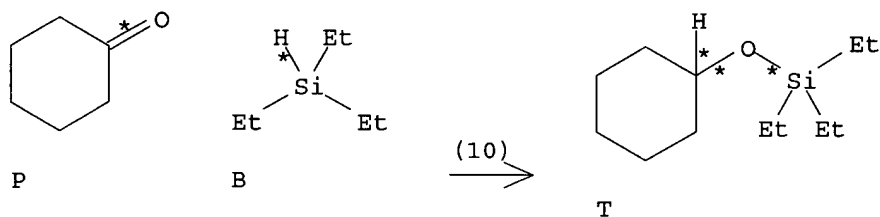
RX (6) RCT J 627-19-0, B 617-86-7
 PRO K 68928-08-5, L 68928-07-4, M 40962-02-5
 CAT 12246-51-4 Cyclooctene Ir, 603-35-0 PPh3

RX (7) OF 43 3 J + 3 B ==> K + L +
M



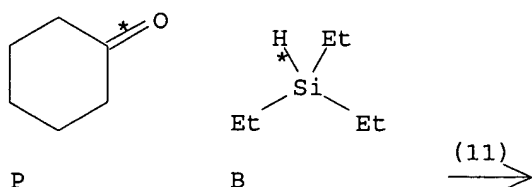
RX (7) RCT J 627-19-0, B 617-86-7
 PRO K 68928-08-5, L 68928-07-4, M
 40962-02-5
 CAT 12246-51-4 Cyclooctene Ir, 6163-58-2
 Tri-o-tolylphosphine

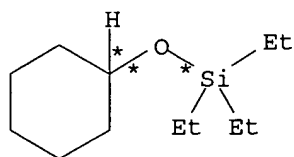
RX (10) OF 43 ...P + B ==> T



RX (10) RCT P 108-94-1, B 617-86-7
 PRO T 4419-18-5
 CAT 12246-51-4 Cyclooctene Ir
 NTE Reaction was run neat

RX (11) OF 43 P + B ==> T

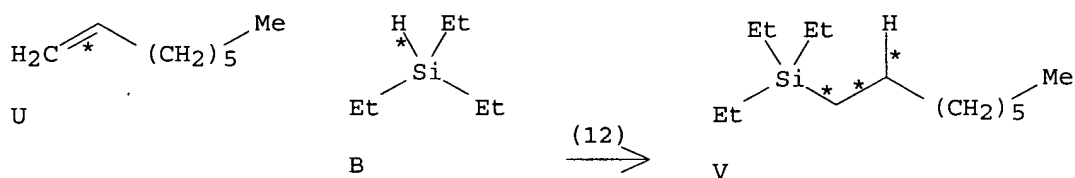




T

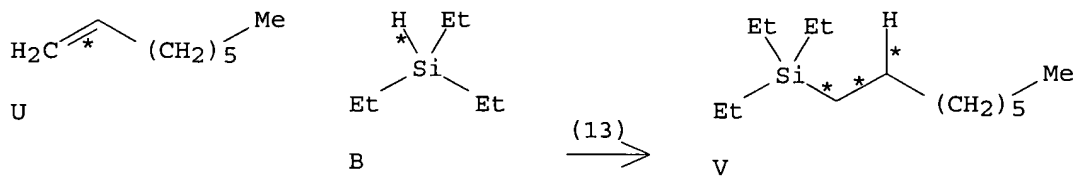
RX(11) RCT P 108-94-1, B 617-86-7
 PRO T 4419-18-5
 CAT 12246-51-4 Cyclooctene Ir, 603-35-0 PPh3
 NTE Reaction was run neat

RX(12) OF 43 U + B ==> V



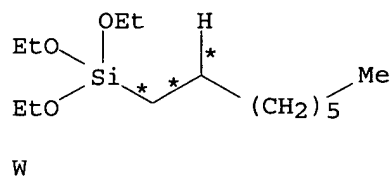
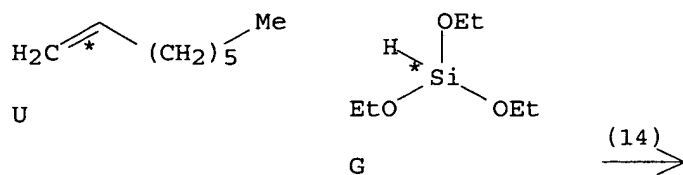
RX(12) RCT U 111-66-0, B 617-86-7
 PRO V 10175-53-8
 CAT 12246-51-4 Cyclooctene Ir, 603-35-0 PPh3
 NTE Rxn was run neat

RX(13) OF 43 U + B ==> V



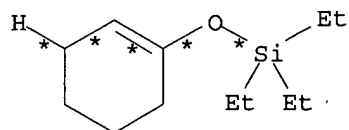
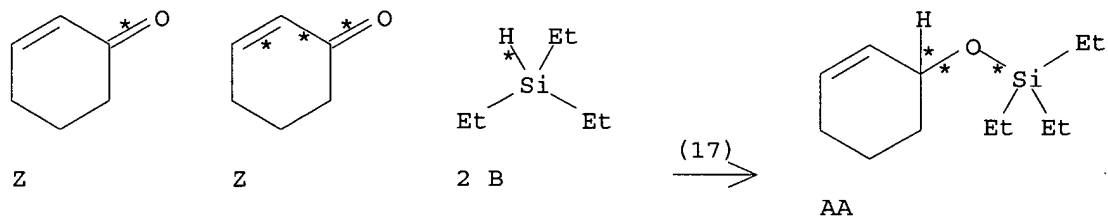
RX(13) RCT U 111-66-0, B 617-86-7
 PRO V 10175-53-8
 CAT 12246-51-4 Cyclooctene Ir, 6163-58-2
 Tri-o-tolylphosphine
 NTE Rxn was run neat

RX(14) OF 43 U + G ==> W



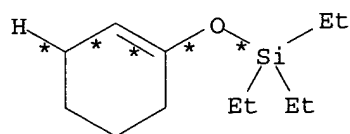
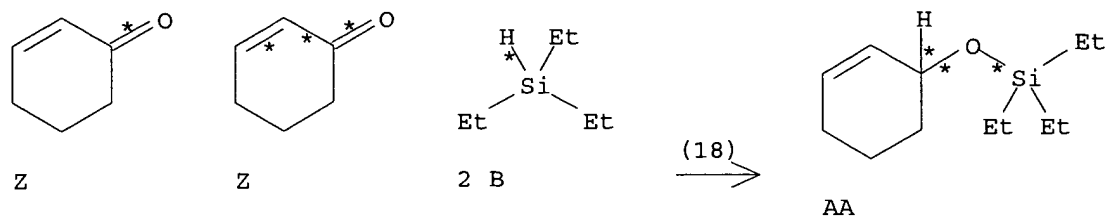
RX(14) RCT U 111-66-0, G 998-30-1
 PRO W 2943-75-1
 CAT 12246-51-4 Cyclooctene Ir, 603-35-0 PPh3
 NTE Rxn was run neat

RX(17) OF 43 2 Z + 2 B ==> AA + O...



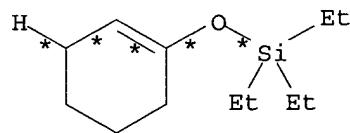
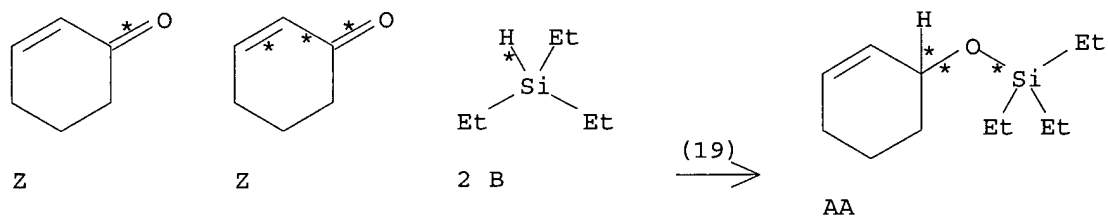
RX(17) RCT Z 930-68-7, B 617-86-7
 PRO AA 96474-45-2, O 4342-22-7
 CAT 12246-51-4 Cyclooctene Ir
 NTE The rxn was run neat. The 1,2-adduct was the major product

RX(18) OF 43 2 Z + 2 B ==> AA + O



O

RX(18) RCT Z 930-68-7, B 617-86-7
 PRO AA 96474-45-2, O 4342-22-7
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η) -
 1,5-cyclooctadiene]di-
 NTE The rxn was run neat. The 1,2-adduct was the major product

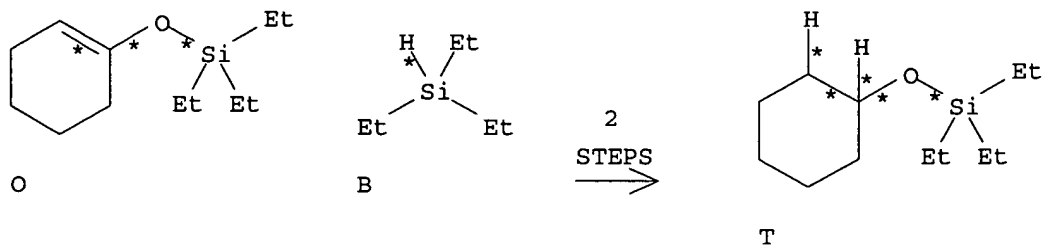
$$\text{RX (19) OF 43} \quad 2 \text{ Z} + 2 \text{ B} \implies \text{AA} + \text{O}$$


0

RX(19) RCT Z 930-68-7, B 617-86-7
PRO AA 96474-45-2, O 4342-22-7
CAT 12246-51-4 Cyclooctene Ir, 603-35-0 PPh3
NTE The rxn was run neat. The 1,4-adduct was the major product

RX(31) OF 43 COMPOSED OF RX(8), RX(10)

RX(31) O + B ==> T

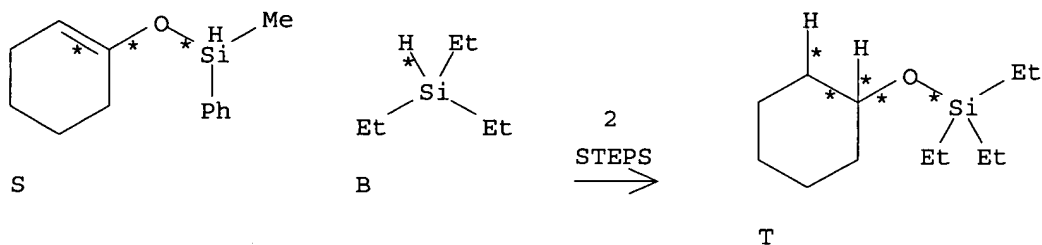


RX(8) RCT O 4342-22-7
 RGT Q 584-08-7 K2CO3
 PRO P 108-94-1
 SOL 67-56-1 MeOH

RX(10) RCT P 108-94-1, B 617-86-7
 PRO T 4419-18-5
 CAT 12246-51-4 Cyclooctene Ir
 NTE Reaction was run neat

RX(33) OF 43 COMPOSED OF RX(9), RX(10)

RX(33) S + B ==> T

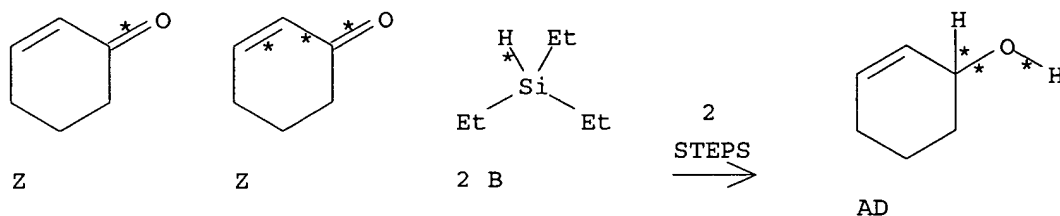


RX(9) RCT S 70790-00-0
 RGT Q 584-08-7 K2CO3
 PRO P 108-94-1
 SOL 67-56-1 MeOH

RX(10) RCT P 108-94-1, B 617-86-7
 PRO T 4419-18-5
 CAT 12246-51-4 Cyclooctene Ir
 NTE Reaction was run neat

RX(35) OF 43 COMPOSED OF RX(17), RX(21)

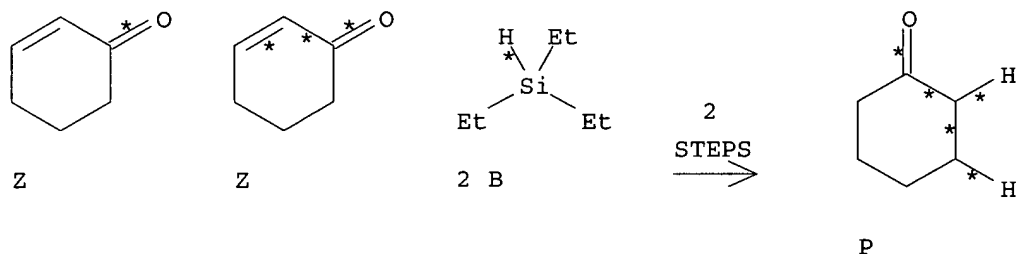
RX(35) 2 Z + 2 B ==> AD



RX(17) RCT Z 930-68-7, B **617-86-7**
 PRO AA 96474-45-2, O 4342-22-7
 CAT **12246-51-4** Cyclooctene Ir
 NTE The rxn was run neat. The 1,2-adduct was the major product

RX(21) RCT AA 96474-45-2
 RGT Q 584-08-7 K₂CO₃
 PRO AD **822-67-3**
 SOL 67-56-1 MeOH

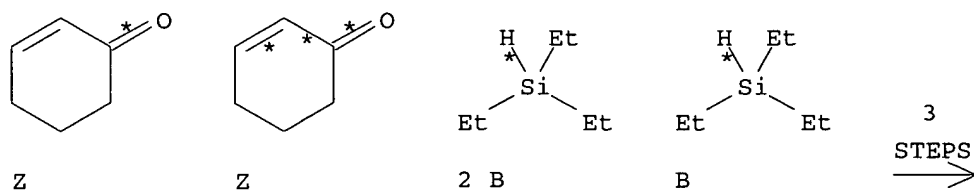
RX(36) OF 43 COMPOSED OF RX(17), RX(8)
 RX(36) 2 Z + 2 B ==> P

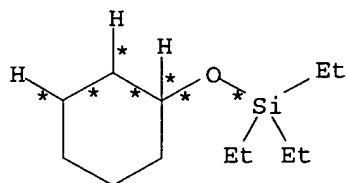


RX(17) RCT Z 930-68-7, B **617-86-7**
 PRO AA 96474-45-2, O 4342-22-7
 CAT **12246-51-4** Cyclooctene Ir
 NTE The rxn was run neat. The 1,2-adduct was the major product

RX(8) RCT O 4342-22-7
 RGT Q 584-08-7 K₂CO₃
 PRO P **108-94-1**
 SOL 67-56-1 MeOH

RX(40) OF 43 COMPOSED OF RX(17), RX(8), RX(10)
 RX(40) 2 Z + 3 B ==> T





T

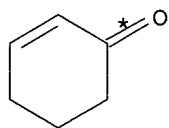
RX(17) RCT Z 930-68-7, B **617-86-7**
 PRO AA 96474-45-2, O 4342-22-7
 CAT **12246-51-4** Cyclooctene Ir
 NTE The rxn was run neat. The 1,2-adduct was the major product

RX(8) RCT O 4342-22-7
 RGT Q 584-08-7 K₂CO₃
 PRO P 108-94-1
 SOL 67-56-1 MeOH

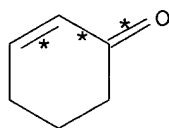
RX(10) RCT P 108-94-1, B **617-86-7**
 PRO T **4419-18-5**
 CAT **12246-51-4** Cyclooctene Ir
 NTE Reaction was run neat

RX(41) OF 43 COMPOSED OF RX(17), RX(8), RX(28)

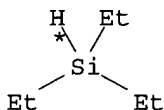
RX(41) 2 Z + 4 B + 2 F + E ==> T + AS



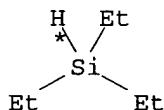
Z



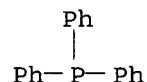
Z



2 B



2 B



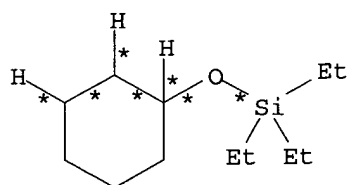
2 F

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

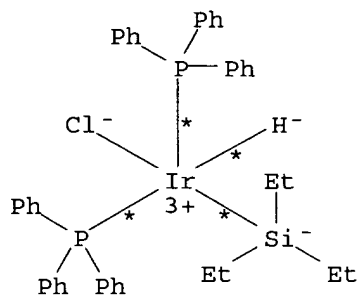
3

STEPS

→



T



AS

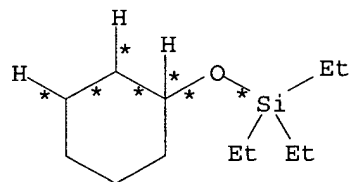
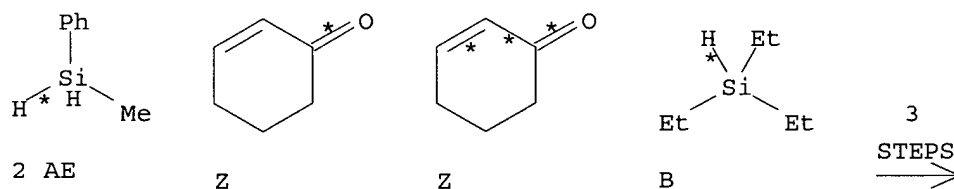
RX(17) RCT Z 930-68-7, B **617-86-7**
 PRO AA 96474-45-2, O 4342-22-7
 CAT **12246-51-4** Cyclooctene Ir
 NTE The rxn was run neat. The 1,2-adduct was the major product

RX(8) RCT O 4342-22-7
 RGT Q 584-08-7 K₂CO₃
 PRO P 108-94-1
 SOL 67-56-1 MeOH

RX(28) RCT P 108-94-1, B **617-86-7**, F 603-35-0, E 12246-51-4
 PRO T **4419-18-5**, AS **75661-49-3**
 NTE Only 2% of the hydrosilation product forms

RX(42) OF 43 COMPOSED OF RX(22), RX(9), RX(10)

RX(42) 2 AE + 2 Z + B ==> T



T

RX(22) RCT AE 766-08-5, Z 930-68-7
 PRO AC 96474-46-3, S 70790-00-0
 CAT **12246-51-4** Cyclooctene Ir, 603-35-0 PPh₃

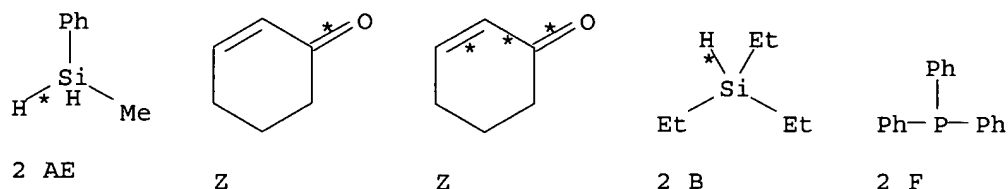
NTE The rxn was run neat. The 1,2-adduct was the major product

RX(9) RCT S 70790-00-0
 RGT Q 584-08-7 K₂CO₃
 PRO P 108-94-1
 SOL 67-56-1 MeOH

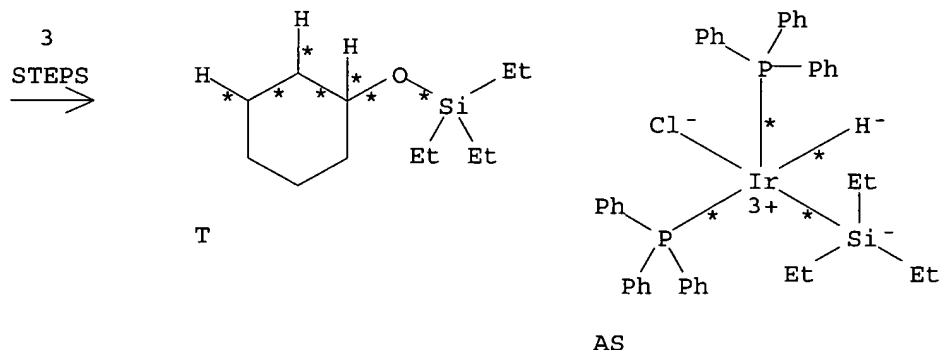
RX(10) RCT P 108-94-1, B 617-86-7
 PRO T 4419-18-5
 CAT 12246-51-4 Cyclooctene Ir
 NTE Reaction was run neat

RX(43) OF 43 COMPOSED OF RX(22), RX(9), RX(28)

RX(43) 2 AE + 2 Z + 2 B + 2 F + E ==> T +
 AS



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



RX(22) RCT AE 766-08-5, Z 930-68-7
 PRO AC 96474-46-3, S 70790-00-0
 CAT 12246-51-4 Cyclooctene Ir, 603-35-0 PPh₃
 NTE The rxn was run neat. The 1,2-adduct was the major product

RX(9) RCT S 70790-00-0
 RGT Q 584-08-7 K₂CO₃
 PRO P 108-94-1
 SOL 67-56-1 MeOH

RX(28) RCT P 108-94-1, B 617-86-7, F 603-35-0, E 12246-51-4
 PRO T 4419-18-5, AS 75661-49-3
 NTE Only 2% of the hydrosilation product forms

L64 ANSWER 15 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:373443 CASREACT

TITLE: Catalytic reductive alkylation of secondary amine with aldehyde and silane by an iridium compound

AUTHOR(S): Mizuta, Tomoya; Sakaguchi, Satoshi; Ishii, Yasutaka

CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering High Technology Research Center, Kansai University, Suita, Osaka, 564-8680, Japan

SOURCE: Journal of Organic Chemistry (2005), 70(6), 2195-2199

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

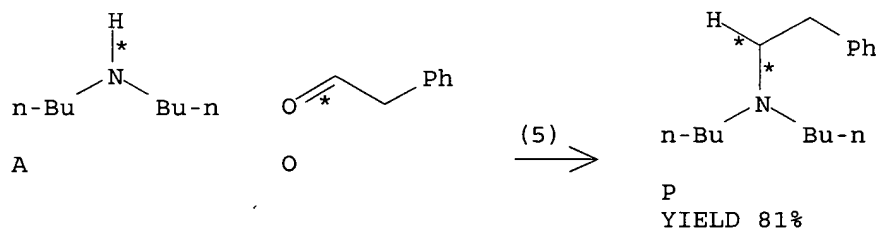
DOCUMENT TYPE: Journal

LANGUAGE: English

AB An efficient methodol. for the reductive alkylation of secondary amine with aldehyde and Et₃SiH using an iridium complex as a catalyst has been developed. Treatment of dibutylamine with butyraldehyde and Et₃SiH under the influence of a catalytic amount of [IrCl(cod)]₂ gave tributylamine in quant. yield. In this reaction, no reduction of aldehyde took place. It was found that IrCl₃, which was a starting material for preparation of iridium complexes such as [IrCl(cod)]₂, acted as an efficient catalyst for the present reductive alkylation of amine. In addition, a cheaper, easy-to-handle, and environmentally friendly reducing reagent such as polymethylhydrosiloxane (PMHS) in place of Et₃SiH was also useful. Thus, a variety of secondary amines could be alkylated by allowing them to react with aldehydes and PMHS in the presence of an iridium catalyst to afford the corresponding tertiary amines in good to excellent yields. From the deuterium label expts., it was revealed that silane and water, generated during the formation of enamine by the reaction of amine and aldehyde, behave as a hydrogen source. The catalytic cycle is also discussed.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(5) OF 12 A + O ==> P



RX(5) RCT A 111-92-2, O 122-78-1

STAGE(1)

RGT Q 617-86-7 Et₃SiH

CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-

SOL 123-91-1 Dioxane

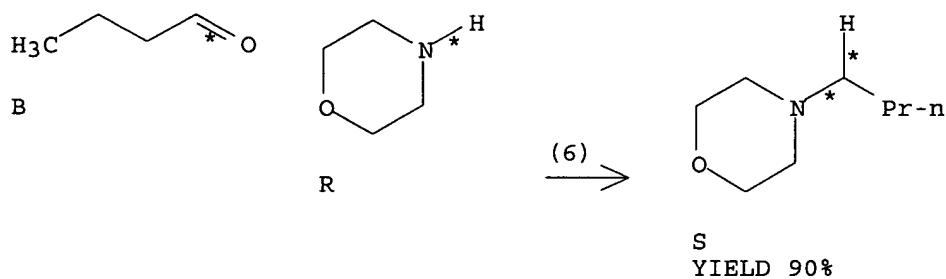
CON 5 hours, 50 deg C

STAGE(2)

RGT E 7732-18-5 Water, F 60-29-7 Et₂O

PRO P 5779-51-1

RX(6) OF 12 B + R ==> S



RX(6) RCT B 123-72-8, R 110-91-8

STAGE(1)

RGT Q 617-86-7 Et₃SiH

CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-

SOL 123-91-1 Dioxane

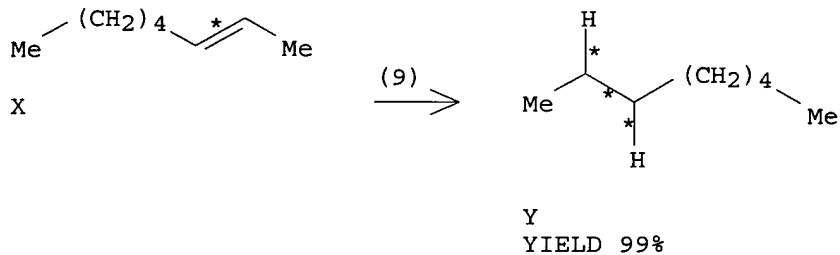
CON 8 hours, 75 deg C

STAGE(2)

RGT E 7732-18-5 Water, F 60-29-7 Et₂O

PRO S 1005-67-0

RX(9) OF 12 X ==> Y



RX(9) RCT X 111-67-1

RGT Q 617-86-7 Et₃SiH, E 7732-18-5 Water

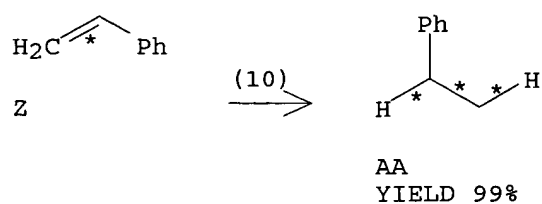
PRO Y 111-65-9

CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-

SOL 123-91-1 Dioxane

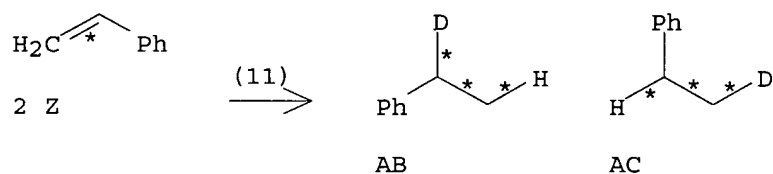
CON 8 hours, 75 deg C

RX(10) OF 12 Z ==> AA



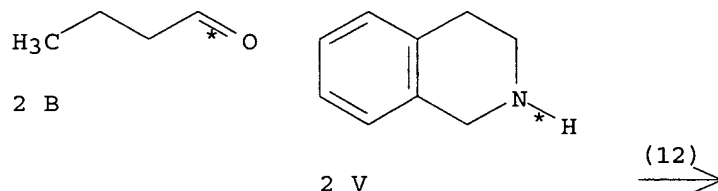
RX(10) RCT Z 100-42-5
 RGT Q 617-86-7 Et3SiH, E 7732-18-5 Water
 PRO AA 100-41-4
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-
 1,5-cyclooctadiene]di-
 SOL 123-91-1 Dioxane
 CON 8 hours, 75 deg C

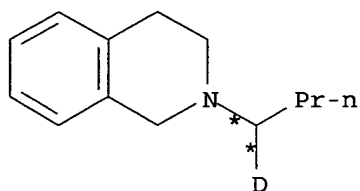
RX(11) OF 12 2 Z ==> AB + AC



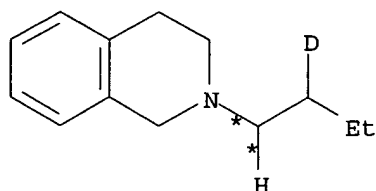
RX(11) RCT Z 100-42-5
 RGT Q 617-86-7 Et3SiH, AD 7789-20-0 D2O
 PRO AB 1861-02-5, AC 1861-04-7
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-
 1,5-cyclooctadiene]di-
 SOL 123-91-1 Dioxane
 CON 8 hours, 75 deg C

RX(12) OF 12 2 B + 2 V ==> AE + AF





AE



AF

RX(12) RCT B 123-72-8, V 91-21-4

STAGE(1)

RGT AG 1631-33-0 Silane-d, triethyl-
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-
 η)-1,5-cyclooctadiene]di-
 SOL 123-91-1 Dioxane
 CON 5 hours, 50 deg C

STAGE(2)

RGT E 7732-18-5 Water, F 60-29-7 Et₂O

PRO AE 849592-25-2, AF 849592-26-3

L64 ANSWER 16 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:447278 CASREACT

TITLE: Organosilanols as Catalysts in Asymmetric Aryl
 Transfer Reactions

AUTHOR(S): Oezcubukcu, Salih; Schmidt, Frank; Bolm, Carsten

CORPORATE SOURCE: Institut fuer Organische Chemie, RWTH Aachen, Aachen,
 D-52074, Germany

SOURCE: Organic Letters (2005), 7(7), 1407-1409

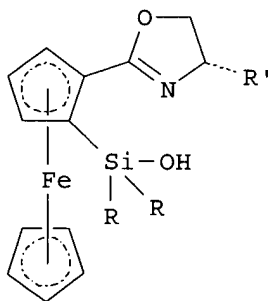
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



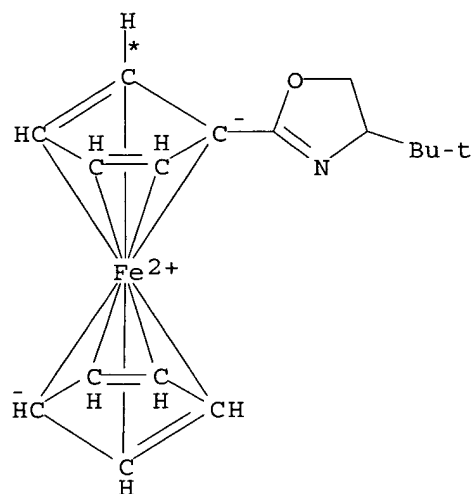
I

AB Various ferrocene-based organosilanols (I, R = CH₃, i-Pr, Ph; R' = t-Bu, Ph, i-Pr, CH₂Ph) have been synthesized in four steps starting from achiral ferrocene carboxylic acid. Applying these novel planar-chiral ferrocenes as catalysts in asym. Ph transfer reactions to substituted benzaldehydes afforded products with high enantiomeric excesses. The best result (91% ee) was achieved in the addition to p-chlorobenzaldehyde with organosilanol I (R = i-Pr, R' = t-Bu), which has a tert-Bu substituent on the oxazoline ring and an iso-Pr group on the silanol fragment.

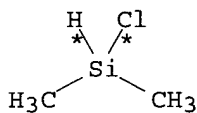
REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(23) OF 29 COMPOSED OF RX(1), RX(8)

RX(23) A + B ==> R



A



B

2
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 162157-02-0

STAGE(1)

RGT D 598-30-1 s-BuLi

SOL 109-99-9 THF, 110-82-7 Cyclohexane

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> -78 deg C

SUBSTAGE(3) 2 hours, -78 deg C

STAGE(2)

RCT B 1066-35-9

CON overnight, -78 deg C -> room temperature

PRO C 851192-07-9

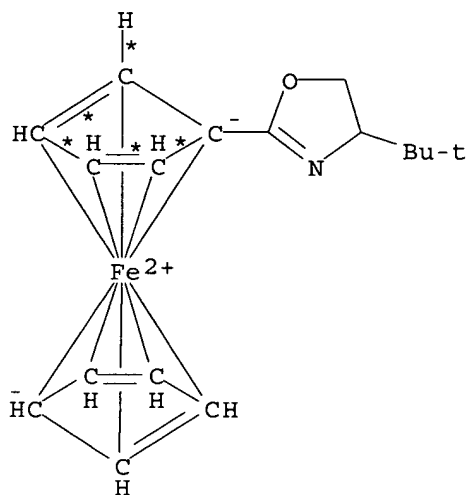
NTE stereoselective

RX(8) RCT C 851192-07-9

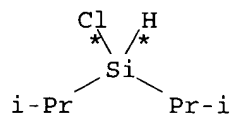
RGT S 7732-18-5 Water, T 7782-44-7 O2
 PRO R 851192-16-0
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-
 1,5-cyclooctadiene]di-
 SOL 75-05-8 MeCN
 CON room temperature
 NTE stereoselective

RX(24) OF 29 COMPOSED OF RX(2), RX(9)

RX(24) A + G ==> W

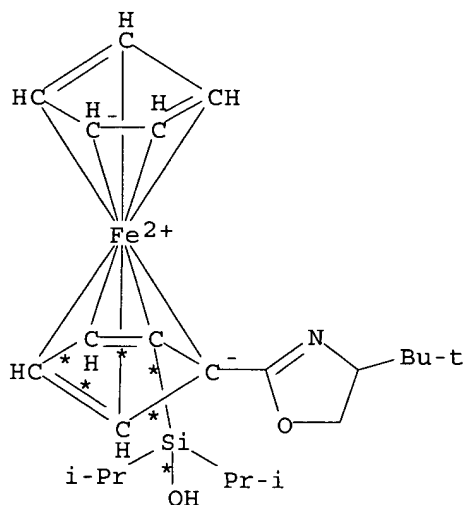


A



G

2
STEPS
→



W

YIELD 77%

RX(2) RCT A 162157-02-0

STAGE(1)

RGT D 598-30-1 s-BuLi
 SOL 109-99-9 THF, 110-82-7 Cyclohexane
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> -78 deg C
 SUBSTAGE(3) 2 hours, -78 deg C

STAGE(2)

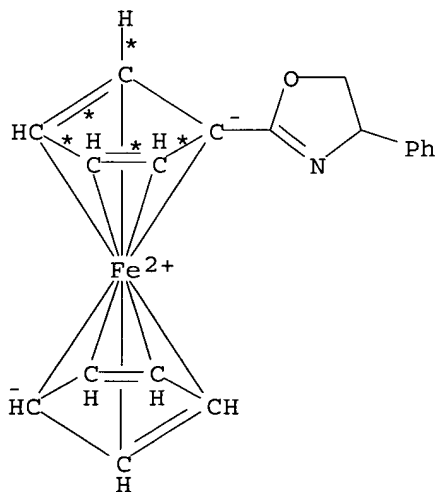
RCT G 2227-29-4
 CON overnight, -78 deg C -> room temperature

PRO H 851192-08-0
 NTE stereoselective

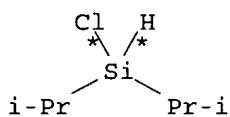
RX(9) RCT H 851192-08-0
 RGT S 7732-18-5 Water, T 7782-44-7 O2
 PRO W 851192-18-2
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-
 SOL 75-05-8 MeCN
 CON 60 deg C
 NTE stereoselective

RX(26) OF 29 COMPOSED OF RX(4), RX(11)

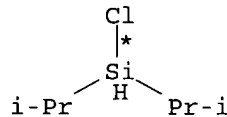
RX(26) 2 K + 2 G ==> Y



2 K

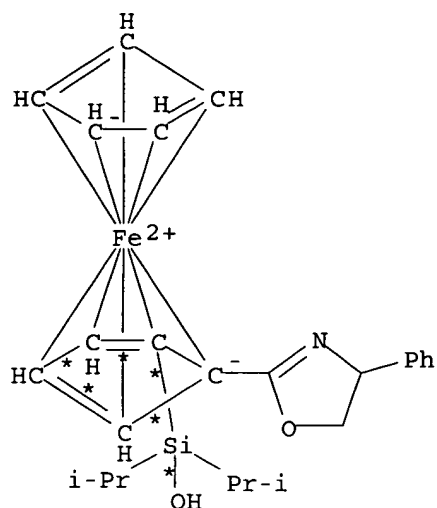


G



G

2
STEPS
→



Y
YIELD 57%

RX(4) RCT K 162157-04-2

STAGE(1)

RGT D 598-30-1 s-BuLi
SOL 109-99-9 THF, 110-82-7 Cyclohexane
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C
SUBSTAGE(3) 2 hours, -78 deg C

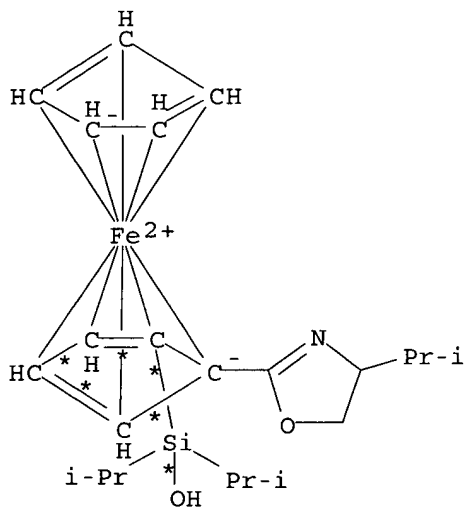
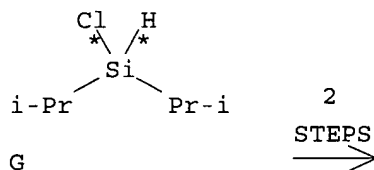
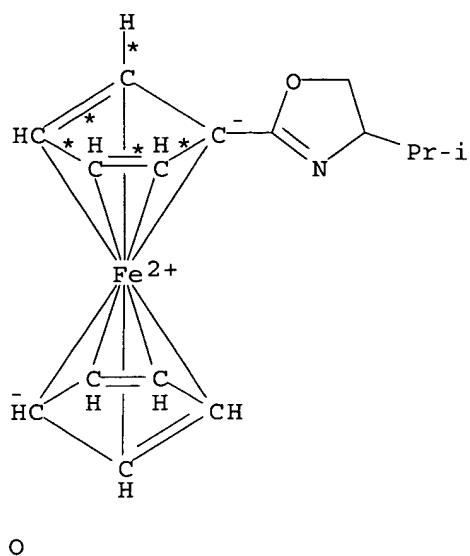
STAGE(2)

RCT G 2227-29-4
CON overnight, -78 deg C -> room temperature

PRO L 851192-10-4, M 851192-34-2
NTE 70% overall yield, stereoselective

RX(11) RCT L 851192-10-4
RGT S 7732-18-5 Water, T 7782-44-7 O2
PRO Y 851192-23-9
CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 75-05-8 MeCN
CON 60 deg C
NTE stereoselective

RX(28) OF 29 COMPOSED OF RX(6), RX(13)
RX(28) O + G ==> AA



YIELD 65%

RX(6) RCT O 162157-03-1

STAGE(1)

RGT D 598-30-1 s-BuLi
 SOL 109-99-9 THF, 110-82-7 Cyclohexane
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> -78 deg C
 SUBSTAGE(3) 2 hours, -78 deg C

STAGE(2)

RCT G 2227-29-4

CON overnight, -78 deg C -> room temperature

PRO P 851192-12-6
NTE stereoselective

RX(13) RCT P 851192-12-6
RGT S 7732-18-5 Water, T 7782-44-7 O2
PRO AA 851192-26-2
CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-
SOL 75-05-8 MeCN
CON room temperature
NTE stereoselective

L64 ANSWER 17 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 140:287436 CASREACT

TITLE: Highly Efficient Iridium-Catalyzed Oxidation of Organosilanes to Silanols

AUTHOR(S): Lee, Youngjun; Seomoon, Dong; Kim, Sundae; Han, Hoon; Chang, Sukbok; Lee, Phil Ho

CORPORATE SOURCE: Department of Chemistry, Kangwon National University, Chuncheon, 200-701, S. Korea

SOURCE: Journal of Organic Chemistry (2004), 69(5), 1741-1743
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

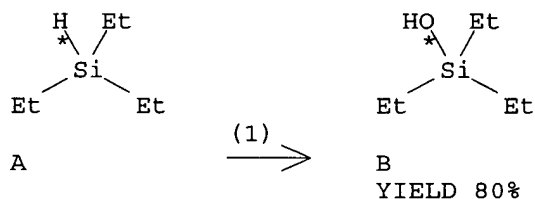
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Hydrolytic oxidation of organosilanes to the corresponding silanols can be performed highly efficiently with a catalyst system of $[\text{IrCl}(\text{C}_8\text{H}_{12})]_2$ under essentially neutral and mild conditions, and various types of silanols are produced in good to excellent yields. Oxidation of silanes $\text{R}_1\text{R}_2\text{R}_3\text{SiH}$ by exposure to air in the presence of 1 mol% of $[\text{IrCl}(\text{cod})]_2$ (cod = 1,2,5,6- η -1,5-cyclooctadiene) gave silanols $\text{R}_1\text{R}_2\text{R}_3\text{SiOH}$ ($\text{R}_1\text{R}_2\text{R}_3$ = Et₃, iBu₃, Ph₃, PhMe₂, Ph₂Me, Ph₂H; R_1 = R_2 = Me, R_3 = C₁₈H₃₇, 4-MeOC₆H₄, 4-BuC₆H₄, 4-MeC₆H₄CH₂, PhCH:CH, Cl(CH₂)₃C.tplbond.C, 2-thienyl, 3-quinoliny1; R_1 = R_2 = iPr, R_3 = PhC.tplbond.C; R_1 = R_2 = Ph, R_3 = 2-thienyl) with yields generally higher than 80%. Oxidation of (+)-methyl(1-naphthyl)phenylsilane gave corresponding silanol with almost complete racemization.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

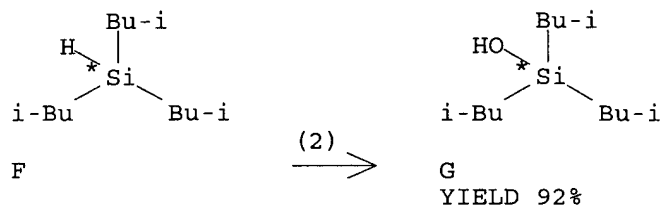
RX(1) OF 18 A ==> B



RX(1) RCT A 617-86-7
RGT C 7732-18-5 Water
PRO B 597-52-4
CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-

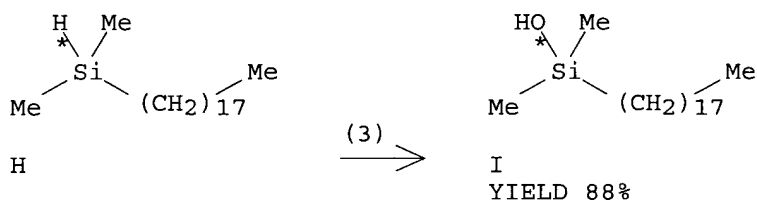
1,5-cyclooctadiene]di-
 SOL 75-05-8 MeCN
 CON 4 hours, room temperature
 NTE alternative reaction conditions gave lower yield

RX(2) OF 18 **F** ==> **G**



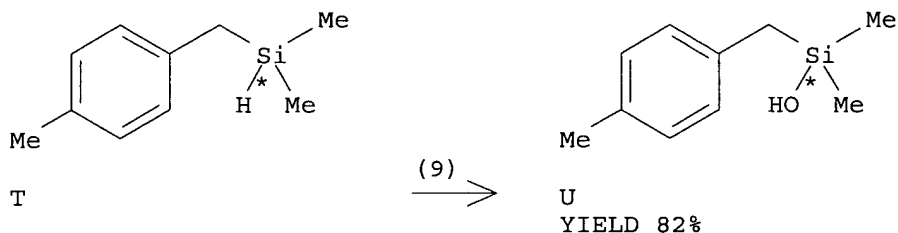
RX(2) RCT **F 6485-81-0**
 RGT **C 7732-18-5** Water
 PRO **G 317374-14-4**
 CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-
 1,5-cyclooctadiene]di-
 SOL 75-05-8 MeCN
 CON 2 hours, 80 deg C

RX(3) OF 18 **H** ==> **I**



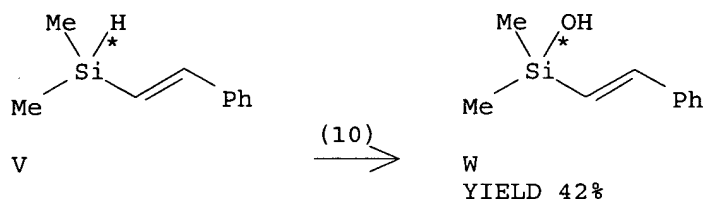
RX(3) RCT **H 32395-58-7**
 RGT **C 7732-18-5** Water
 PRO **I 58626-12-3**
 CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-
 1,5-cyclooctadiene]di-
 SOL 75-05-8 MeCN
 CON 3 hours, room temperature

RX(9) OF 18 **T** ==> **U**



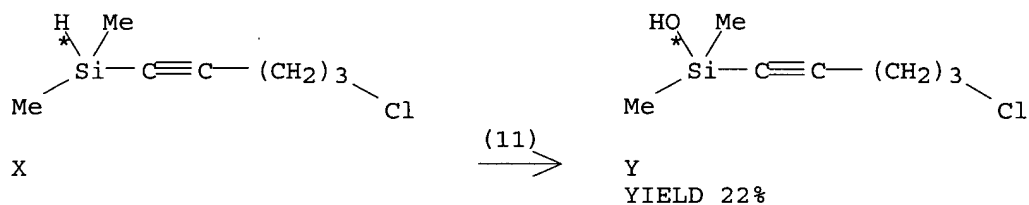
RX(9) RCT T 27856-33-3
 RGT C 7732-18-5 Water
 PRO U 70430-64-7
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-
 SOL 75-05-8 MeCN
 CON 0.5 hours, room temperature

RX(10) OF 18 V ==> W



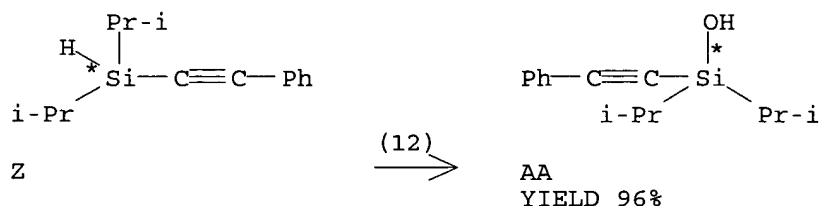
RX(10) RCT V 119873-75-5
 RGT C 7732-18-5 Water
 PRO W 119873-74-4
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-
 SOL 75-05-8 MeCN
 CON 0.5 hours, room temperature

RX(11) OF 18 X ==> Y



RX(11) RCT X 317374-20-2
 RGT C 7732-18-5 Water
 PRO Y 317374-16-6
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-
 SOL 75-05-8 MeCN
 CON 0.5 hours, room temperature

RX(12) OF 18 Z ==> AA

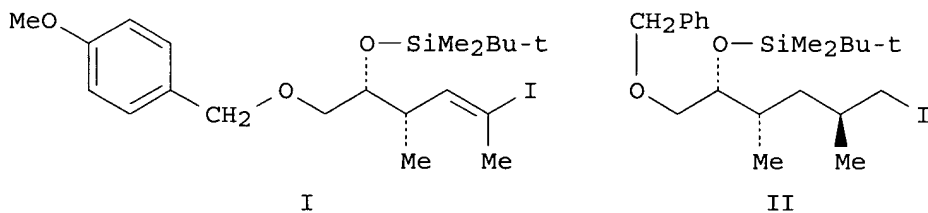


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RX(12)      RCT  Z 317374-19-9
            RGT  C 7732-18-5 Water
            PRO  AA 317374-15-5
            CAT  12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-
            1,5-cyclooctadiene]di-
            SOL  75-05-8 MeCN
            CON  12 hours, room temperature

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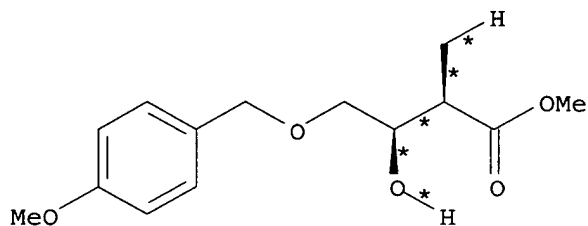
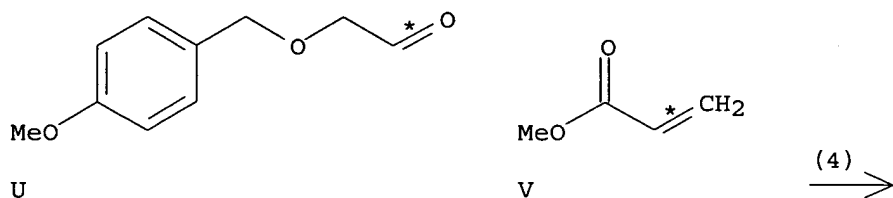
L64 ANSWER 18 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 138:237929 CASREACT
TITLE: Enantioselective Total Synthesis of Borrelidin
AUTHOR(S): Duffey, Matthew O.; LeTiran, Arnaud; Morken, James P.
CORPORATE SOURCE: Department of Chemistry Venable and Kenan
Laboratories, University of North Carolina at Chapel
Hill, Chapel Hill, NC, 27599-3290, USA
SOURCE: Journal of the American Chemical Society (2003),
125(6), 1458-1459
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The first total synthesis of the natural product borrelidin is described. The propionate fragment of the mol. was concisely synthesized through catalytic enantioselective reductive aldol reactions, a catalytic Negishi coupling of vinyl iodide I with alkyl iodide II, and a catalytic directed hydrogenation. The propionate segment was then fused to the vinyl iodide fragment through a catalytic Sonogashira coupling. Subsequent catalytic hydrostannylation and catalytic cyanation allowed access to the target structure.

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX (4) OF 594 U + V ==> W...



YIELD 76%

RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, 12112-67-3
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH₂CH₂Cl
CON 1 hour, room temperature

STAGE(2)

RGT X 760-32-7 MeEt₂SiH
SOL 107-06-2 ClCH₂CH₂Cl
CON 30 minutes, room temperature

STAGE(3)

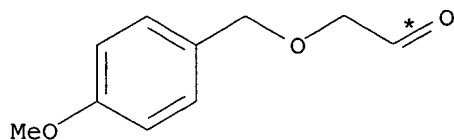
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH₂CH₂Cl
CON 48 hours, room temperature

STAGE(4)

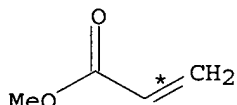
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

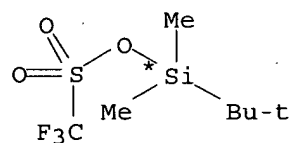
RX(50) OF 594 COMPOSED OF RX(4), RX(16)
RX(50) U + V + BY ==> BZ



U

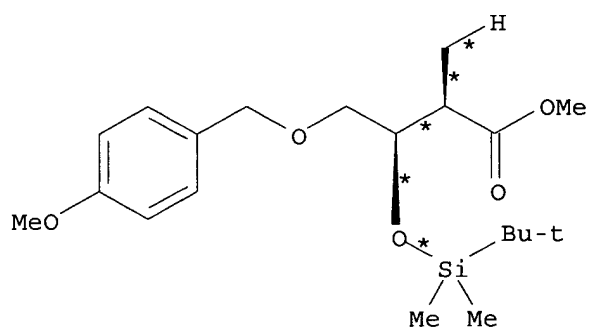


V



BY

2
STEPS
→



BZ

YIELD 90%

RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, 12112-67-3
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)

RGT X 760-32-7 MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)

RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

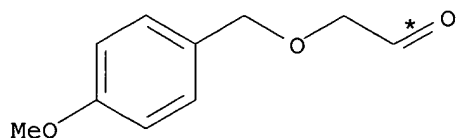
STAGE(3)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

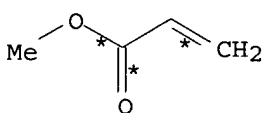
PRO BZ 501419-19-8

RX(98) OF 594 COMPOSED OF RX(4), RX(16), RX(17)

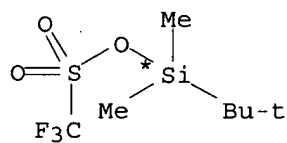
RX(98) U + V + BY ==> CB



U

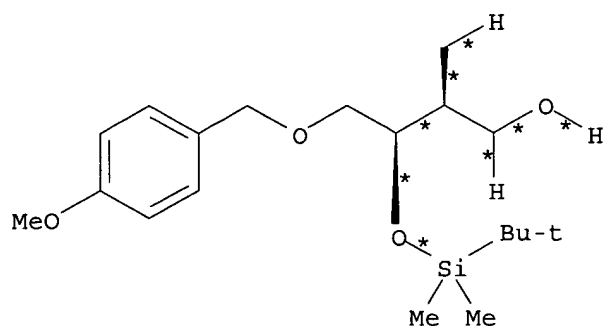


V



BY

3
STEPS
→



CB
YIELD 79%

RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, 12112-67-3
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH₂CH₂Cl
CON 1 hour, room temperature

STAGE(2)

RGT X 760-32-7 MeEt₂SiH
SOL 107-06-2 ClCH₂CH₂Cl
CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH₂CH₂Cl
CON 48 hours, room temperature

STAGE(4)

RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 15 minutes, 0 deg C

SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)2
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)

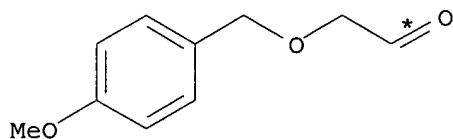
RGT O 67-56-1 MeOH

STAGE(3)

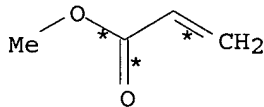
RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

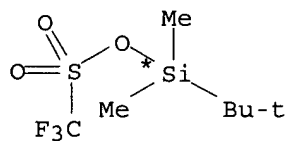
RX(119) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18)
RX(119) U + V + BY ==> CD



U

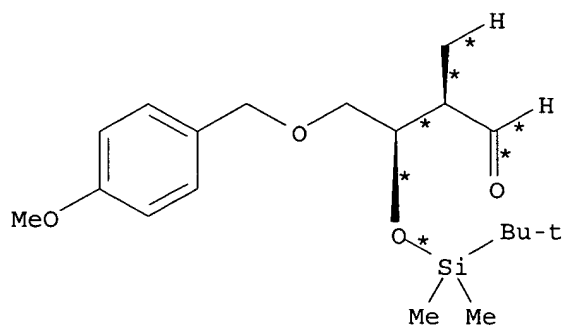


V



BY

4
STEPS
→



CD
YIELD 92%

RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3a α ,8a α]]-, **12112-67-3**
Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH₂CH₂Cl
CON 1 hour, room temperature

STAGE(2)

RGT X **760-32-7** MeEt₂SiH
SOL 107-06-2 ClCH₂CH₂Cl
CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH₂CH₂Cl
CON 48 hours, room temperature

STAGE(4)

RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 15 minutes, 0 deg C

SUBSTAGE(2) 0 deg C -> room temperature
 SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT G 144-55-8 NaHCO3
 SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)2
 SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
 CON SUBSTAGE(1) -78 deg C
 SUBSTAGE(2) 45 minutes, -78 deg C
 SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)

RGT O 67-56-1 MeOH

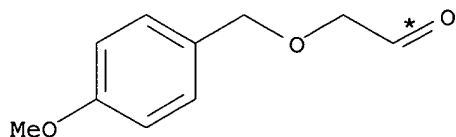
STAGE(3)

RGT CC 304-59-6 Rochelle salt
 SOL 7732-18-5 Water

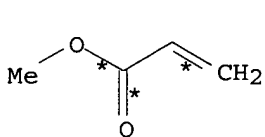
PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
 RGT CE 87413-09-0 Martin's reagent
 PRO CD 501419-21-2
 SOL 75-09-2 CH2Cl2
 CON 90 minutes, room temperature

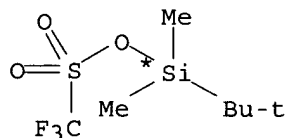
RX(195) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19)
 RX(195) U + V + BY + CF ==> CG



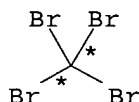
U



V

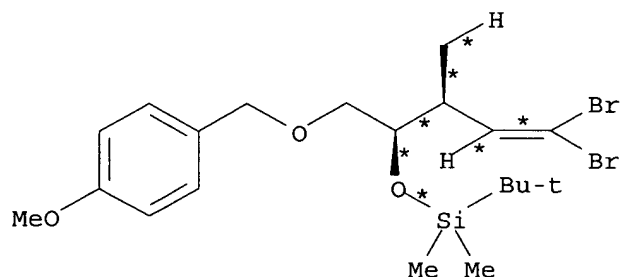


BY



CF

5
 STEPS
 —————>



CG
YIELD 94%

RX (4)

STAGE (1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3a α ,8a α]]-, 12112-67-3
Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH₂CH₂Cl
CON 1 hour, room temperature

STAGE (2)

RGT X 760-32-7 MeEt₂SiH
SOL 107-06-2 ClCH₂CH₂Cl
CON 30 minutes, room temperature

STAGE (3)

RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH₂CH₂Cl
CON 48 hours, room temperature

STAGE (4)

RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX (16) RCT W 501419-01-8

STAGE (1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE (1) room temperature
SUBSTAGE (2) room temperature -> 0 deg C

STAGE (2)

RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE (1) 15 minutes, 0 deg C
SUBSTAGE (2) 0 deg C -> room temperature
SUBSTAGE (3) 1 hour, room temperature

STAGE(3)

RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)2
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)

RGT O 67-56-1 MeOH

STAGE(3)

RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH2Cl2
CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)

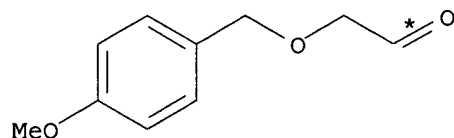
RGT AI 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)

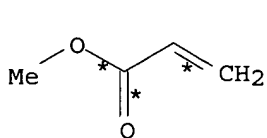
RCT CD 501419-21-2
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 30 minutes, -78 deg C
SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

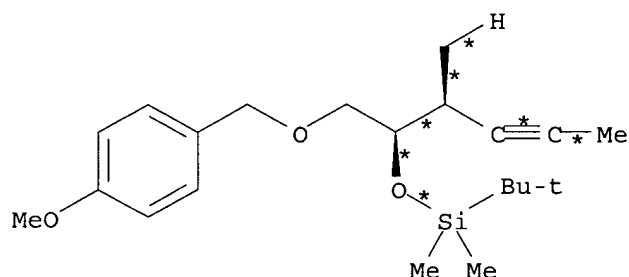
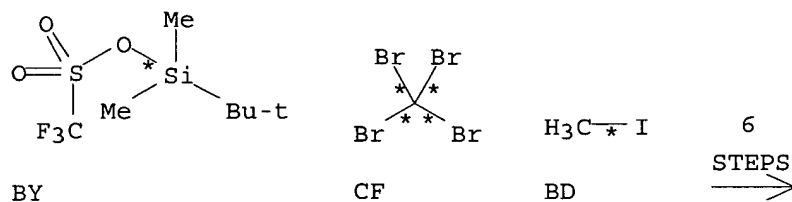
RX(270) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20)
RX(270) U + V + BY + CF + BD ==> AB



U



V



AB
YIELD 97%

RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, 12112-67-3
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH₂CH₂Cl
CON 1 hour, room temperature

STAGE(2)

RGT X 760-32-7 MeEt₂SiH
SOL 107-06-2 ClCH₂CH₂Cl
CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH₂CH₂Cl
CON 48 hours, room temperature

STAGE(4)

RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)₂
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)

RGT O 67-56-1 MeOH

STAGE(3)

RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)

RGT AI 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)

RCT CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 30 minutes, -78 deg C
SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

RX(20) RCT CG 501419-22-3

STAGE(1)

RGT CH 109-72-8 BuLi
 SOL 109-99-9 THF, 110-54-3 Hexane
 CON SUBSTAGE(1) -78 deg C
 SUBSTAGE(2) -78 deg C -> -25 deg C
 SUBSTAGE(3) 1 hour, -25 deg C
 SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)

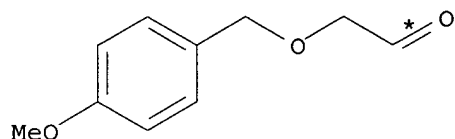
RCT BD 74-88-4
 SOL 109-99-9 THF
 CON SUBSTAGE(1) -78 deg C
 SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)

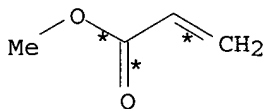
RGT AQ 12125-02-9 NH4Cl
 SOL 7732-18-5 Water

PRO AB 501419-23-4

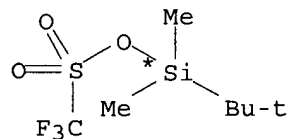
RX(273) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20), RX(5)
 RX(273) U + V + BY + CF + BD ==> AC



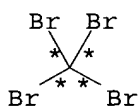
U



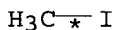
V



BY

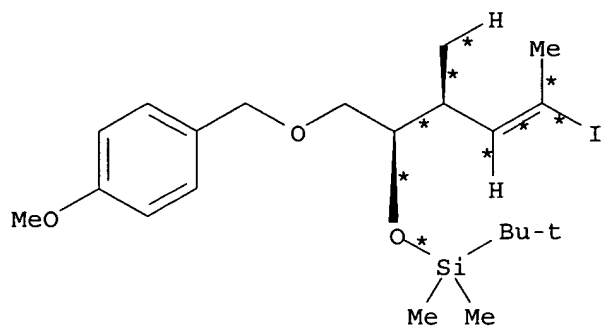


CF



BD

7
 STEPS
 →



AC
YIELD 89%

RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3a α ,8a α]]-, 12112-67-3
Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH₂CH₂Cl
CON 1 hour, room temperature

STAGE(2)

RGT X 760-32-7 MeEt₂SiH
SOL 107-06-2 ClCH₂CH₂Cl
CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH₂CH₂Cl
CON 48 hours, room temperature

STAGE(4)

RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 15 minutes, 0 deg C

SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)₂
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)

RGT O 67-56-1 MeOH

STAGE(3)

RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)

RGT AI 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)

RCT CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 30 minutes, -78 deg C
SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

RX(20) RCT CG 501419-22-3

STAGE(1)

RGT CH 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -25 deg C
SUBSTAGE(3) 1 hour, -25 deg C
SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)

RCT BD 74-88-4
 SOL 109-99-9 THF
 CON SUBSTAGE(1) -78 deg C
 SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)

RGT AQ 12125-02-9 NH4Cl
 SOL 7732-18-5 Water

PRO AB 501419-23-4

RX(5) RCT AB 501419-23-4

STAGE(1)

RGT AD 37342-97-5 Hydrozirconocene Cl
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 2 hours, room temperature
 SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

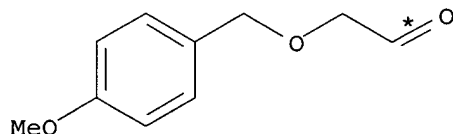
RGT AE 7553-56-2 I2
 SOL 56-23-5 CCl4
 CON 0 deg C

PRO AC 501419-02-9

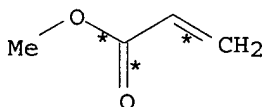
NTE in the dark, regioselective, stereoselective

RX(277) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20),
 RX(5), RX(9)

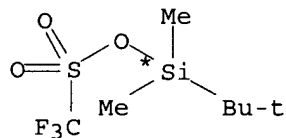
RX(277) U + V + BY + CF + BD + AT ==> AU



U



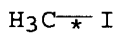
V



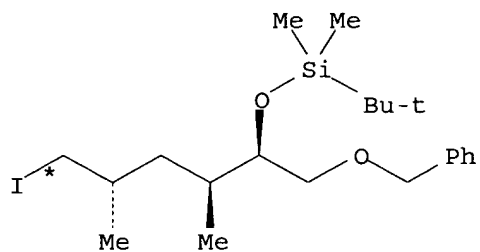
BY



CF

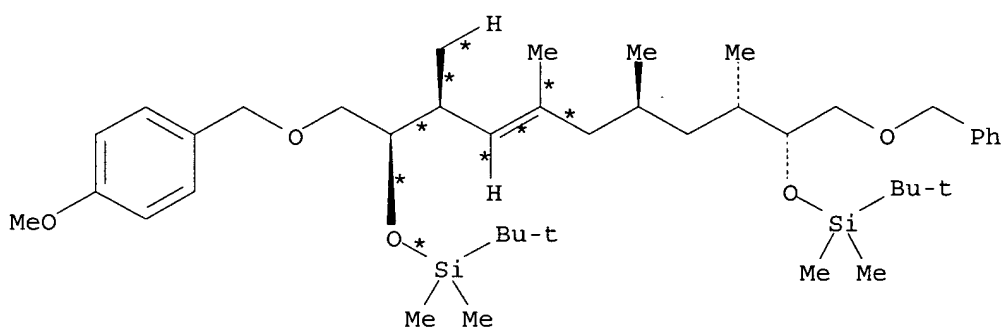


BD



AT

8
STEPS
→



AU

YIELD 58%

RX (4)

STAGE (1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, 12112-67-3
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH₂CH₂Cl
CON 1 hour, room temperature

STAGE (2)

RGT X 760-32-7 MeEt₂SiH
SOL 107-06-2 ClCH₂CH₂Cl
CON 30 minutes, room temperature

STAGE (3)

RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH₂CH₂Cl
CON 48 hours, room temperature

STAGE (4)

RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)
RGT BF 1191-15-7 AlH(Bu-i)₂
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)
RGT O 67-56-1 MeOH

STAGE(3)
RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)
RGT AI 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)
RCT CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) -78 deg C

SUBSTAGE(2) 30 minutes, -78 deg C
SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

RX(20) RCT CG 501419-22-3

STAGE(1)

RGT CH 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -25 deg C
SUBSTAGE(3) 1 hour, -25 deg C
SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)

RCT BD 74-88-4
SOL 109-99-9 THF
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)

RGT AQ 12125-02-9 NH4Cl
SOL 7732-18-5 Water

PRO AB 501419-23-4

RX(5) RCT AB 501419-23-4

STAGE(1)

RGT AD 37342-97-5 Hydrozirconocene Cl
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 2 hours, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RGT AE 7553-56-2 I2
SOL 56-23-5 CCl4
CON 0 deg C

PRO AC 501419-02-9

NTE in the dark, regioselective, stereoselective

RX(9) RCT AT 501419-06-3

STAGE(1)

RGT AV 7646-85-7 ZnCl2
SOL 60-29-7 Et2O
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C

STAGE(2)

RGT AW 594-19-4 t-BuLi
SOL 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 5 minutes, -78 deg C
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RCT AC 501419-02-9

CAT 14221-01-3 Pd(PPh₃)₄
 CON 16 hours, room temperature

STAGE(4)

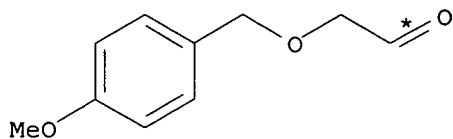
RGT K 7732-18-5 Water
 SOL 7732-18-5 Water

PRO AU 501419-08-5

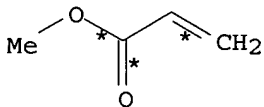
NTE modified Negishi coupling, stage three in the dark

RX(386) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20),
 RX(5), RX(9), RX(24)

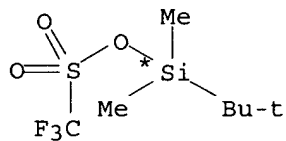
RX(386) U + V + BY + CF + BD + AT ==> AY



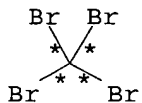
U



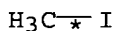
V



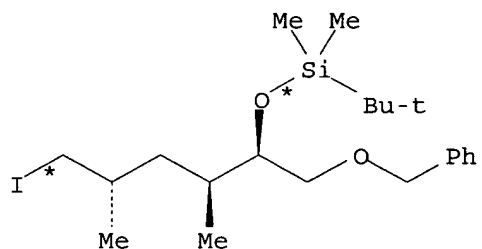
BY



CF

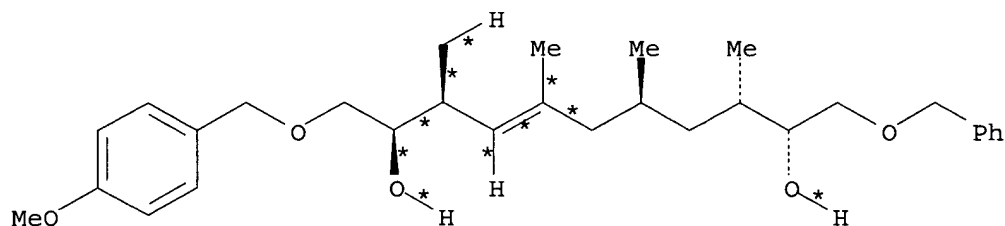


BD



AT

9
 STEPS
 →



AY
YIELD 87%

RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, 12112-67-3
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH₂CH₂Cl
CON 1 hour, room temperature

STAGE(2)

RGT X 760-32-7 MeEt₂SiH
SOL 107-06-2 ClCH₂CH₂Cl
CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH₂CH₂Cl
CON 48 hours, room temperature

STAGE(4)

RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)₂
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)

RGT O 67-56-1 MeOH

STAGE(3)

RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)

RGT AI 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)

RCT CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 30 minutes, -78 deg C
SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

RX(20) RCT CG 501419-22-3

STAGE(1)

RGT CH 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -25 deg C
SUBSTAGE(3) 1 hour, -25 deg C
SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)

RCT BD 74-88-4
SOL 109-99-9 THF
CON SUBSTAGE(1) -78 deg C

SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)

RGT AQ 12125-02-9 NH₄Cl
SOL 7732-18-5 Water

PRO AB 501419-23-4

RX(5) RCT AB 501419-23-4

STAGE(1)

RGT AD 37342-97-5 Hydrozirconocene Cl
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 2 hours, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RGT AE 7553-56-2 I₂
SOL 56-23-5 CCl₄
CON 0 deg C

PRO AC 501419-02-9

NTE in the dark, regioselective, stereoselective

RX(9) RCT AT 501419-06-3

STAGE(1)

RGT AV 7646-85-7 ZnCl₂
SOL 60-29-7 Et₂O
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C

STAGE(2)

RGT AW 594-19-4 t-BuLi
SOL 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 5 minutes, -78 deg C
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RCT AC 501419-02-9
CAT 14221-01-3 Pd(PPh₃)₄
CON 16 hours, room temperature

STAGE(4)

RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO AU 501419-08-5

NTE modified Negishi coupling, stage three in the dark

RX(24) RCT AU 501419-08-5

RGT CM 429-41-4 Bu₄N.F

PRO AY 501419-27-8

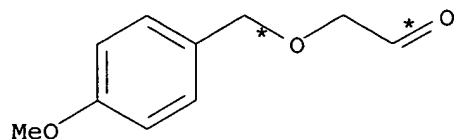
SOL 109-99-9 THF

CON 20 hours, room temperature

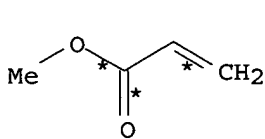
NTE mol. sieves

RX(414) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20),

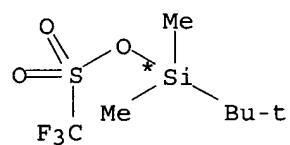
RX(5), RX(9), RX(24), RX(10), RX(25), RX(26)
 RX(414) U + V + 3 BY + CF + BD + AT ==> CO



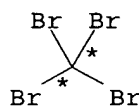
U



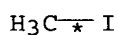
V



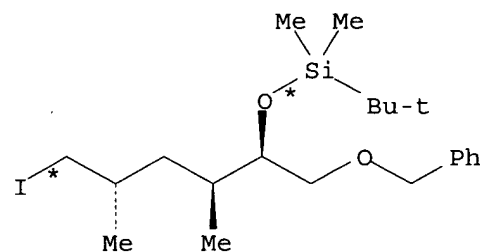
3 BY



CF

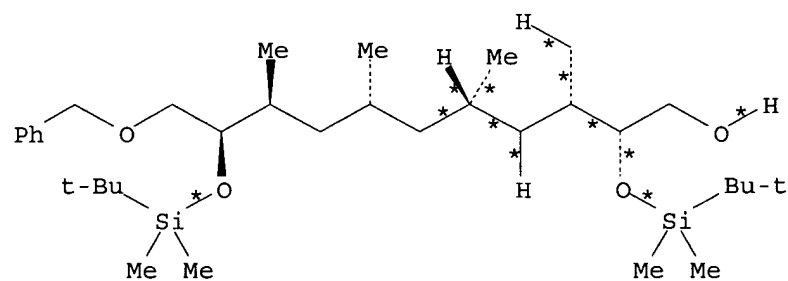


BD



AT

12
STEPS
→



CO
YIELD 93%

RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-

[2 (3aR*,8aS*),3a α ,8a α]]-, 12112-67-3
Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-
cyclooctadiene]di-

SOL 107-06-2 ClCH₂CH₂Cl
CON 1 hour, room temperature

STAGE(2)

RGT X 760-32-7 MeEt₂SiH
SOL 107-06-2 ClCH₂CH₂Cl
CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH₂CH₂Cl
CON 48 hours, room temperature

STAGE(4)

RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)₂
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)

RGT O 67-56-1 MeOH

STAGE(3)

RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)
RGT AI 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)
RCT CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 30 minutes, -78 deg C
SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

RX(20) RCT CG 501419-22-3

STAGE(1)
RGT CH 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -25 deg C
SUBSTAGE(3) 1 hour, -25 deg C
SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)
RCT BD 74-88-4
SOL 109-99-9 THF
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)
RGT AQ 12125-02-9 NH₄Cl
SOL 7732-18-5 Water

PRO AB 501419-23-4

RX(5) RCT AB 501419-23-4

STAGE(1)
RGT AD 37342-97-5 Hydrozirconocene Cl
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 2 hours, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RGT AE 7553-56-2 I₂
SOL 56-23-5 CCl₄
CON 0 deg C

PRO AC 501419-02-9
NTE in the dark, regioselective, stereoselective

RX(9) RCT AT 501419-06-3

STAGE(1)
RGT AV 7646-85-7 ZnCl₂
SOL 60-29-7 Et₂O
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C

STAGE(2)
RGT AW 594-19-4 t-BuLi
SOL 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 5 minutes, -78 deg C
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RCT AC 501419-02-9
CAT 14221-01-3 Pd(PPh₃)₄
CON 16 hours, room temperature

STAGE(4)
RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO AU 501419-08-5
NTE modified Negishi coupling, stage three in the dark

RX(24) RCT AU 501419-08-5
RGT CM 429-41-4 Bu₄N.F
PRO AY 501419-27-8
SOL 109-99-9 THF
CON 20 hours, room temperature
NTE mol. sieves

RX(10) RCT AY 501419-27-8
RGT BA 1333-74-0 H₂
PRO AZ 501419-10-9
CAT 82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-dienel [1,4-butanediylbis[diphenylphosphine-κP]]-, tetrafluoroborate(1-)
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 4 hours, room temperature, 700 psi
NTE high pressure, stereoselective

RX(25) RCT AZ 501419-10-9, BY 69739-34-0

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature -> 0 deg C
SUBSTAGE(2) 5 minutes, 0 deg C
SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

STAGE(2)
RGT G 144-55-8 NaHCO₃

SOL 7732-18-5 Water

PRO CN 501419-28-9

RX(26) RCT CN 501419-28-9

STAGE(1)

RGT CP 84-58-2 DDQ

SOL 75-09-2 CH₂Cl₂, 7732-18-5 Water

CON 1 hour, room temperature, pH 7

STAGE(2)

RGT G 144-55-8 NaHCO₃

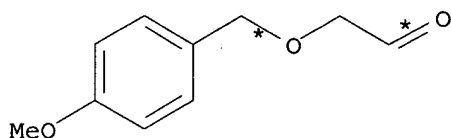
SOL 7732-18-5 Water

PRO CO 501419-29-0

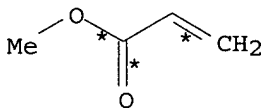
NTE chemoselective, buffered soln.

RX(415) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20),
 RX(5), RX(9), RX(24), RX(10), RX(25), RX(26), RX(27)

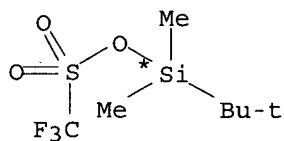
RX(415) U + V + 3 BY + CF + BD + AT + CQ ==> CR



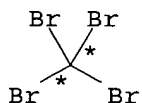
U



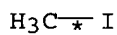
V



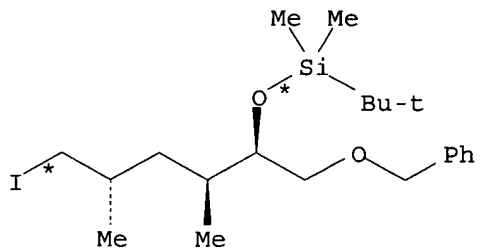
3 BY



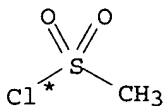
CF



BD

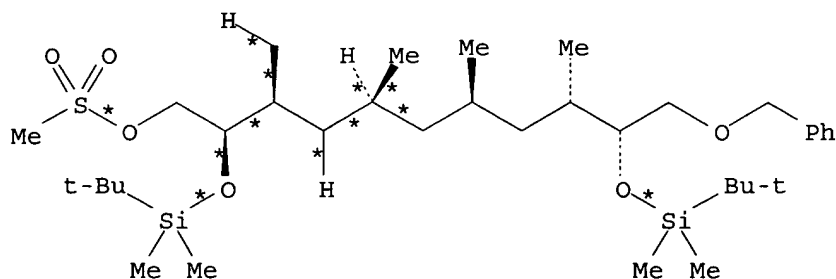


AT



CQ

13
 STEPS
 →



CR

RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, 12112-67-3
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH₂CH₂Cl
CON 1 hour, room temperature

STAGE(2)

RGT X 760-32-7 MeEt₂SiH
SOL 107-06-2 ClCH₂CH₂Cl
CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH₂CH₂Cl
CON 48 hours, room temperature

STAGE(4)

RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT G 144-55-8 NaHCO₃

SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)₂SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane

CON SUBSTAGE(1) -78 deg C

SUBSTAGE(2) 45 minutes, -78 deg C

SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)

RGT O 67-56-1 MeOH

STAGE(3)

RGT CC 304-59-6 Rochelle salt

SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1

RGT CE 87413-09-0 Martin's reagent

PRO CD 501419-21-2

SOL 75-09-2 CH₂Cl₂

CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)

RGT AI 603-35-0 PPh₃SOL 75-09-2 CH₂Cl₂

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)

RCT CD 501419-21-2

SOL 75-09-2 CH₂Cl₂

CON SUBSTAGE(1) -78 deg C

SUBSTAGE(2) 30 minutes, -78 deg C

SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

RX(20) RCT CG 501419-22-3

STAGE(1)

RGT CH 109-72-8 BuLi

SOL 109-99-9 THF, 110-54-3 Hexane

CON SUBSTAGE(1) -78 deg C

SUBSTAGE(2) -78 deg C -> -25 deg C

SUBSTAGE(3) 1 hour, -25 deg C

SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)

RCT BD 74-88-4

SOL 109-99-9 THF

CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)
RGT AQ 12125-02-9 NH₄Cl
SOL 7732-18-5 Water

PRO AB 501419-23-4

RX(5) RCT AB 501419-23-4

STAGE(1)
RGT AD 37342-97-5 Hydrozirconocene Cl
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 2 hours, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RGT AE 7553-56-2 I₂
SOL 56-23-5 CCl₄
CON 0 deg C

PRO AC 501419-02-9
NTE in the dark, regioselective, stereoselective

RX(9) RCT AT 501419-06-3

STAGE(1)
RGT AV 7646-85-7 ZnCl₂
SOL 60-29-7 Et₂O
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C

STAGE(2)
RGT AW 594-19-4 t-BuLi
SOL 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 5 minutes, -78 deg C
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RCT AC 501419-02-9
CAT 14221-01-3 Pd(PPh₃)₄
CON 16 hours, room temperature

STAGE(4)
RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO AU 501419-08-5
NTE modified Negishi coupling, stage three in the dark

RX(24) RCT AU 501419-08-5
RGT CM 429-41-4 Bu₄N.F
PRO AY 501419-27-8
SOL 109-99-9 THF
CON 20 hours, room temperature
NTE mol. sieves

RX(10) RCT AY 501419-27-8

RGT BA 1333-74-0 H2
PRO AZ 501419-10-9
CAT 82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene] [1,4-butanediylbis[diphenylphosphine-κP]]-, tetrafluoroborate(1-)
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 4 hours, room temperature, 700 psi
NTE high pressure, stereoselective

RX(25) RCT AZ 501419-10-9, BY 69739-34-0

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature -> 0 deg C
SUBSTAGE(2) 5 minutes, 0 deg C
SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

STAGE(2)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO CN 501419-28-9

RX(26) RCT CN 501419-28-9

STAGE(1)
RGT CP 84-58-2 DDQ
SOL 75-09-2 CH2Cl2, 7732-18-5 Water
CON 1 hour, room temperature, pH 7

STAGE(2)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO CO 501419-29-0
NTE chemoselective, buffered soln.

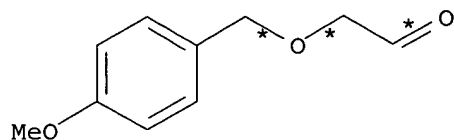
RX(27) RCT CO 501419-29-0, CQ 124-63-0

STAGE(1)
RGT D 121-44-8 Et3N
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C
SUBSTAGE(3) 3 minutes, 0 deg C
SUBSTAGE(4) 1.5 hours, 0 deg C -> room temperature

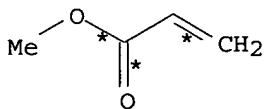
STAGE(2)
RGT K 7732-18-5 Water

PRO CR 501419-30-3

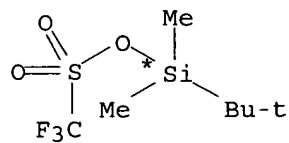
RX(416) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20),
RX(5), RX(9), RX(24), RX(10), RX(25), RX(26), RX(29)
RX(416) U + V + 3 BY + CF + BD + AT ==> CU



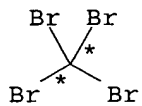
U



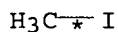
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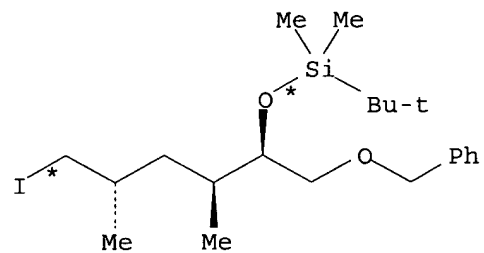
3 BY



CF

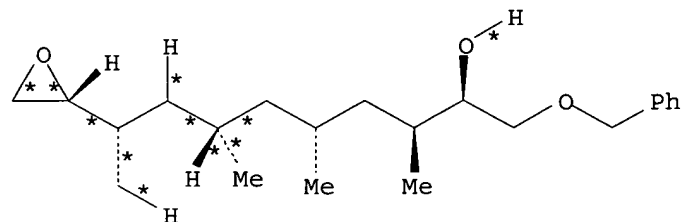


BD



AT

13
STEPS
→



CU
YIELD 98%

RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3**
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH₂CH₂Cl

CON 1 hour, room temperature

STAGE(2)

RGT X 760-32-7 MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)

RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RCT BY 69739-34-0
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)2
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)

RGT O 67-56-1 MeOH

STAGE(3)

RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1

RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)

RGT AI 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)

RCT CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 30 minutes, -78 deg C
SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

RX(20) RCT CG 501419-22-3

STAGE(1)

RGT CH 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -25 deg C
SUBSTAGE(3) 1 hour, -25 deg C
SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)

RCT BD 74-88-4
SOL 109-99-9 THF
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)

RGT AQ 12125-02-9 NH₄Cl
SOL 7732-18-5 Water

PRO AB 501419-23-4

RX(5) RCT AB 501419-23-4

STAGE(1)

RGT AD 37342-97-5 Hydrozirconocene Cl
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 2 hours, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RGT AE 7553-56-2 I₂
SOL 56-23-5 CCl₄
CON 0 deg C

PRO AC 501419-02-9

NTE in the dark, regioselective, stereoselective

RX(9) RCT AT 501419-06-3

STAGE(1)

RGT AV 7646-85-7 ZnCl₂

SOL 60-29-7 Et₂O

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> -78 deg C

STAGE(2)

RGT AW 594-19-4 t-BuLi

SOL 110-54-3 Hexane

CON SUBSTAGE(1) -78 deg C

SUBSTAGE(2) 5 minutes, -78 deg C

SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RCT AC 501419-02-9

CAT 14221-01-3 Pd(PPh₃)₄

CON 16 hours, room temperature

STAGE(4)

RGT K 7732-18-5 Water

SOL 7732-18-5 Water

PRO AU 501419-08-5

NTE modified Negishi coupling, stage three in the dark

RX(24)

RCT AU 501419-08-5

RGT CM 429-41-4 Bu₄N.F

PRO AY 501419-27-8

SOL 109-99-9 THF

CON 20 hours, room temperature

NTE mol. sieves

RX(10)

RCT AY 501419-27-8

RGT BA 1333-74-0 H₂

PRO AZ 501419-10-9

CAT 82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,4-butanediylbis[diphenylphosphine-κP]]-, tetrafluoroborate(1-)

SOL 75-09-2 CH₂Cl₂

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 4 hours, room temperature, 700 psi

NTE high pressure, stereoselective

RX(25)

RCT AZ 501419-10-9, BY 69739-34-0

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine

SOL 75-09-2 CH₂Cl₂

CON SUBSTAGE(1) room temperature -> 0 deg C

SUBSTAGE(2) 5 minutes, 0 deg C

SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

STAGE(2)

RGT G 144-55-8 NaHCO₃

SOL 7732-18-5 Water

PRO CN 501419-28-9

RX(26) RCT CN 501419-28-9

STAGE(1)

RGT CP 84-58-2 DDQ
SOL 75-09-2 CH₂Cl₂, 7732-18-5 Water
CON 1 hour, room temperature, pH 7

STAGE(2)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO CO 501419-29-0
NTE chemoselective, buffered soln.

RX(29) RCT CO 501419-29-0

STAGE(1)

RGT CQ 124-63-0 MeSO₂Cl, D 121-44-8 Et₃N
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C
SUBSTAGE(3) 3 minutes, 0 deg C
SUBSTAGE(4) 1.5 hours, 0 deg C -> room temperature

STAGE(2)

RGT K 7732-18-5 Water

STAGE(3)

RGT CT 7664-39-3 HF
SOL 75-05-8 MeCN, 7732-18-5 Water
CON 3 hours, room temperature

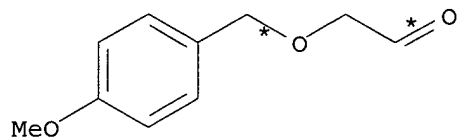
STAGE(4)

RGT BJ 584-08-7 K₂CO₃
SOL 67-56-1 MeOH
CON 45 minutes, room temperature

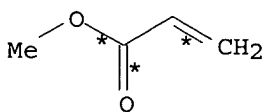
PRO CU 501419-32-5

RX(417) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20),
RX(5), RX(9), RX(24), RX(10), RX(25), RX(26), RX(27), RX(28)

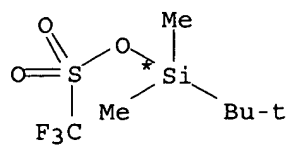
RX(417) U + V + 3 BY + CF + BD + AT + CQ ==> CS



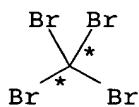
U



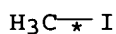
V



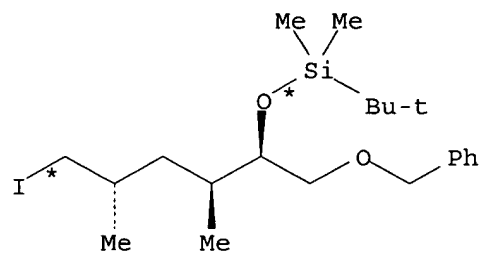
3 BY



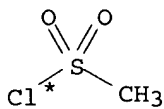
CF



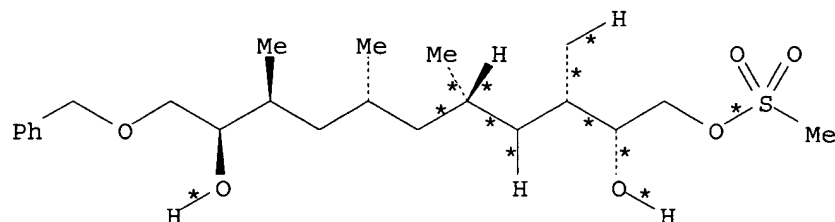
BD



AT



CQ

14
STEPS
→

CS

RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, 12112-67-3
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-

SOL 107-06-2 ClCH₂CH₂Cl

CON 1 hour, room temperature

STAGE(2)

RGT X 760-32-7 MeEt₂SiH

SOL 107-06-2 ClCH₂CH₂Cl

CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3

SOL 107-06-2 ClCH₂CH₂Cl

CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)
RGT BF 1191-15-7 AlH(Bu-i)₂
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)
RGT O 67-56-1 MeOH

STAGE(3)
RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)
RGT AI 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)

RCT CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 30 minutes, -78 deg C
SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

RX(20) RCT CG 501419-22-3

STAGE(1)

RGT CH 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -25 deg C
SUBSTAGE(3) 1 hour, -25 deg C
SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)

RCT BD 74-88-4
SOL 109-99-9 THF
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)

RGT AQ 12125-02-9 NH₄Cl
SOL 7732-18-5 Water

PRO AB 501419-23-4

RX(5) RCT AB 501419-23-4

STAGE(1)

RGT AD 37342-97-5 Hydrozirconocene Cl
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 2 hours, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RGT AE 7553-56-2 I₂
SOL 56-23-5 CCl₄
CON 0 deg C

PRO AC 501419-02-9

NTE in the dark, regioselective, stereoselective

RX(9) RCT AT 501419-06-3

STAGE(1)

RGT AV 7646-85-7 ZnCl₂
SOL 60-29-7 Et₂O
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C

STAGE(2)

RGT AW 594-19-4 t-BuLi
SOL 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C

SUBSTAGE(2) 5 minutes, -78 deg C
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RCT AC 501419-02-9
CAT 14221-01-3 Pd(PPh₃)₄
CON 16 hours, room temperature

STAGE(4)

RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO AU 501419-08-5
NTE modified Negishi coupling, stage three in the dark

RX(24) RCT AU 501419-08-5
RGT CM 429-41-4 Bu₄N.F
PRO AY 501419-27-8
SOL 109-99-9 THF
CON 20 hours, room temperature
NTE mol. sieves

RX(10) RCT AY 501419-27-8
RGT BA 1333-74-0 H₂
PRO AZ 501419-10-9
CAT 82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene] [1,4-butanediylbis[diphenylphosphine-κP]]-, tetrafluoroborate(1-)
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 4 hours, room temperature, 700 psi
NTE high pressure, stereoselective

RX(25) RCT AZ 501419-10-9, BY 69739-34-0

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature -> 0 deg C
SUBSTAGE(2) 5 minutes, 0 deg C
SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

STAGE(2)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO CN 501419-28-9

RX(26) RCT CN 501419-28-9

STAGE(1)

RGT CP 84-58-2 DDQ
SOL 75-09-2 CH₂Cl₂, 7732-18-5 Water
CON 1 hour, room temperature, pH 7

STAGE(2)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO CO 501419-29-0

NTE chemoselective, buffered soln.

RX(27) RCT CO 501419-29-0, CQ 124-63-0

STAGE(1)

RGT D 121-44-8 Et3N

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 0 deg C

SUBSTAGE(3) 3 minutes, 0 deg C

SUBSTAGE(4) 1.5 hours, 0 deg C -> room temperature

STAGE(2)

RGT K 7732-18-5 Water

PRO CR 501419-30-3

RX(28) RCT CR 501419-30-3

RGT CT 7664-39-3 HF

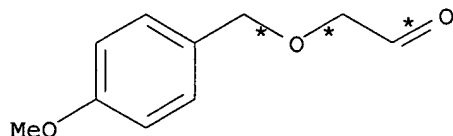
PRO CS 501419-31-4

SOL 75-05-8 MeCN, 7732-18-5 Water

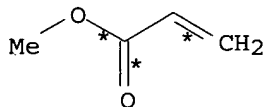
CON 3 hours, room temperature

RX(418) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20),
RX(5), RX(9), RX(24), RX(10), RX(25), RX(26), RX(29), RX(30)

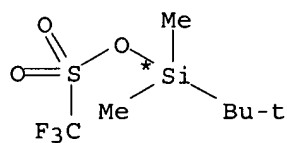
RX(418) U + V + 3 BY + CF + BD + AT + CV ==> CW



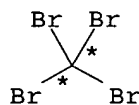
U



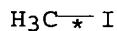
V



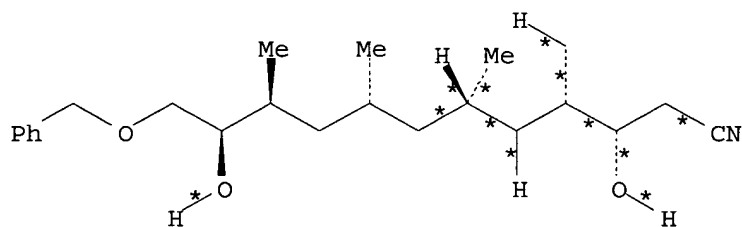
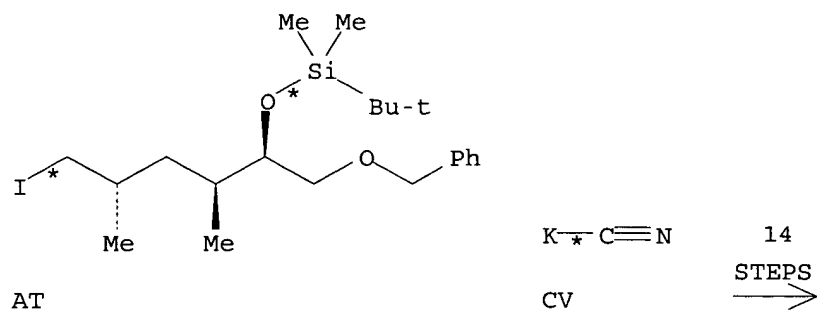
3 BY



CF



BD



RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3**
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH₂CH₂Cl
CON 1 hour, room temperature

STAGE(2)

RGT X **760-32-7** MeEt₂SiH
SOL 107-06-2 ClCH₂CH₂Cl
CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH₂CH₂Cl
CON 48 hours, room temperature

STAGE(4)

RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)₂
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)

RGT O 67-56-1 MeOH

STAGE(3)

RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)

RGT AI 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)

RCT CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 30 minutes, -78 deg C
SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

RX(20) RCT CG 501419-22-3

STAGE(1)

RGT CH 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -25 deg C
SUBSTAGE(3) 1 hour, -25 deg C
SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)

RCT BD 74-88-4
SOL 109-99-9 THF
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)

RGT AQ 12125-02-9 NH4Cl
SOL 7732-18-5 Water

PRO AB 501419-23-4

RX(5) RCT AB 501419-23-4

STAGE(1)

RGT AD 37342-97-5 Hydrozirconocene Cl
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 2 hours, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RGT AE 7553-56-2 I2
SOL 56-23-5 CCl4
CON 0 deg C

PRO AC 501419-02-9

NTE in the dark, regioselective, stereoselective

RX(9) RCT AT 501419-06-3

STAGE(1)

RGT AV 7646-85-7 ZnCl2
SOL 60-29-7 Et2O
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C

STAGE(2)

RGT AW 594-19-4 t-BuLi
SOL 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 5 minutes, -78 deg C
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RCT AC 501419-02-9
CAT 14221-01-3 Pd(PPh3)4
CON 16 hours, room temperature

STAGE(4)

RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO AU 501419-08-5
NTE modified Negishi coupling, stage three in the dark

RX(24) RCT AU 501419-08-5
RGT CM 429-41-4 Bu4N.F
PRO AY 501419-27-8
SOL 109-99-9 THF
CON 20 hours, room temperature
NTE mol. sieves

RX(10) RCT AY 501419-27-8
RGT BA 1333-74-0 H2
PRO AZ 501419-10-9
CAT 82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene] [1,4-butanediylbis[diphenylphosphine-κP]]-, tetrafluoroborate(1-)
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 4 hours, room temperature, 700 psi
NTE high pressure, stereoselective

RX(25) RCT AZ 501419-10-9, BY 69739-34-0

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature -> 0 deg C
SUBSTAGE(2) 5 minutes, 0 deg C
SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

STAGE(2)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO CN 501419-28-9

RX(26) RCT CN 501419-28-9

STAGE(1)
RGT CP 84-58-2 DDQ
SOL 75-09-2 CH2Cl2, 7732-18-5 Water
CON 1 hour, room temperature, pH 7

STAGE(2)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO CO 501419-29-0
NTE chemoselective, buffered soln.

RX(29) RCT CO 501419-29-0

STAGE(1)
RGT CQ 124-63-0 MeSO2Cl, D 121-44-8 Et3N
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

SUBSTAGE(3) 3 minutes, 0 deg C
 SUBSTAGE(4) 1.5 hours, 0 deg C -> room temperature

STAGE(2)

RGT K 7732-18-5 Water

STAGE(3)

RGT CT 7664-39-3 HF
 SOL 75-05-8 MeCN, 7732-18-5 Water
 CON 3 hours, room temperature

STAGE(4)

RGT BJ 584-08-7 K₂CO₃
 SOL 67-56-1 MeOH
 CON 45 minutes, room temperature

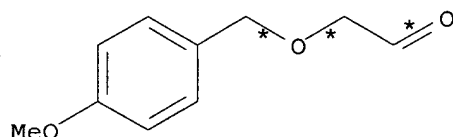
PRO CU 501419-32-5

RX(30) RCT CU 501419-32-5, CV 151-50-8
 PRO CW **501419-33-6**
 SOL 75-05-8 MeCN
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 70 deg C
 SUBSTAGE(3) 24 hours, 70 deg C
 SUBSTAGE(4) 70 deg C -> room temperature

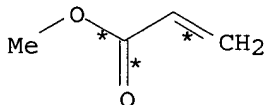
RX(419) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20),
 RX(5), RX(9), RX(24), RX(10), RX(25), RX(26), RX(29), RX(30), RX(31)

RX(419) U + V + 3 BY + CF + BD + AT + CV + 2 CX ==>

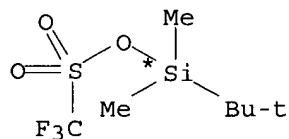
BC



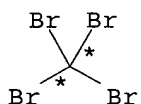
U



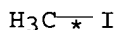
V



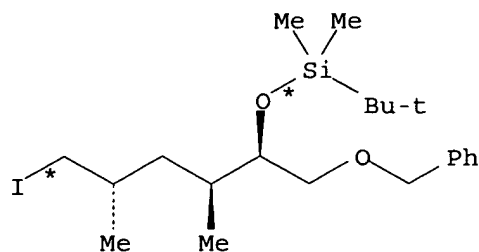
3 BY



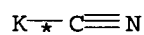
CF



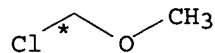
BD



AT

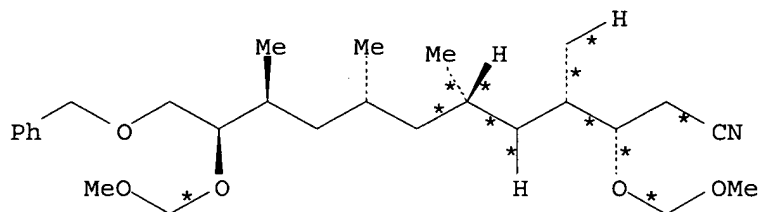


CV



2 CX

15
STEPS
→



BC

YIELD 81%

RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, 12112-67-3
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-

SOL 107-06-2 ClCH₂CH₂Cl

CON 1 hour, room temperature

STAGE(2)

RGT X 760-32-7 MeEt₂SiH

SOL 107-06-2 ClCH₂CH₂Cl

CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3

SOL 107-06-2 ClCH₂CH₂Cl

CON 48 hours, room temperature

STAGE(4)

RGT N 7647-01-0 HCl

SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water

CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)
RGT BF 1191-15-7 AlH(Bu-i)₂
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)
RGT O 67-56-1 MeOH

STAGE(3)
RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)
RGT AI 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)
RCT CD 501419-21-2
SOL 75-09-2 CH₂Cl₂

CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 30 minutes, -78 deg C
SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

RX(20) RCT CG 501419-22-3

STAGE(1)

RGT CH 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -25 deg C
SUBSTAGE(3) 1 hour, -25 deg C
SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)

RCT BD 74-88-4
SOL 109-99-9 THF
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)

RGT AQ 12125-02-9 NH4Cl
SOL 7732-18-5 Water

PRO AB 501419-23-4

RX(5) RCT AB 501419-23-4

STAGE(1)

RGT AD 37342-97-5 Hydrozirconocene Cl
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 2 hours, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RGT AE 7553-56-2 I2
SOL 56-23-5 CCl4
CON 0 deg C

PRO AC 501419-02-9

NTE in the dark, regioselective, stereoselective

RX(9) RCT AT 501419-06-3

STAGE(1)

RGT AV 7646-85-7 ZnCl2
SOL 60-29-7 Et2O
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C

STAGE(2)

RGT AW 594-19-4 t-BuLi
SOL 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 5 minutes, -78 deg C
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RCT AC 501419-02-9
CAT 14221-01-3 Pd(PPh₃)₄
CON 16 hours, room temperature

STAGE(4)

RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO AU 501419-08-5
NTE modified Negishi coupling, stage three in the dark

RX(24) RCT AU 501419-08-5
RGT CM 429-41-4 Bu₄N.F
PRO AY 501419-27-8
SOL 109-99-9 THF
CON 20 hours, room temperature
NTE mol. sieves

RX(10) RCT AY 501419-27-8
RGT BA 1333-74-0 H₂
PRO AZ 501419-10-9
CAT 82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,4-butanediylbis[diphenylphosphine-κP]]-, tetrafluoroborate(1-)
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 4 hours, room temperature, 700 psi
NTE high pressure, stereoselective

RX(25) RCT AZ 501419-10-9, BY 69739-34-0

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature -> 0 deg C
SUBSTAGE(2) 5 minutes, 0 deg C
SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

STAGE(2)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO CN 501419-28-9

RX(26) RCT CN 501419-28-9

STAGE(1)

RGT CP 84-58-2 DDQ
SOL 75-09-2 CH₂Cl₂, 7732-18-5 Water
CON 1 hour, room temperature, pH 7

STAGE(2)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO CO 501419-29-0
NTE chemoselective, buffered soln.

RX(29) RCT CO 501419-29-0

STAGE(1)

RGT CQ 124-63-0 MeSO₂Cl, D 121-44-8 Et₃N
 SOL 75-09-2 CH₂Cl₂
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 0 deg C
 SUBSTAGE(3) 3 minutes, 0 deg C
 SUBSTAGE(4) 1.5 hours, 0 deg C -> room temperature

STAGE(2)

RGT K 7732-18-5 Water

STAGE(3)

RGT CT 7664-39-3 HF
 SOL 75-05-8 MeCN, 7732-18-5 Water
 CON 3 hours, room temperature

STAGE(4)

RGT BJ 584-08-7 K₂CO₃
 SOL 67-56-1 MeOH
 CON 45 minutes, room temperature

PRO CU 501419-32-5

RX(30) RCT CU 501419-32-5, CV 151-50-8
 PRO CW 501419-33-6
 SOL 75-05-8 MeCN
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 70 deg C
 SUBSTAGE(3) 24 hours, 70 deg C
 SUBSTAGE(4) 70 deg C -> room temperature

RX(31) RCT CW 501419-33-6, CX 107-30-2

STAGE(1)

RGT CY 7087-68-5 EtN(Pr-i)₂
 SOL 75-09-2 CH₂Cl₂
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 28 hours, 0 deg C -> room temperature

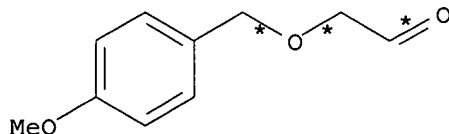
STAGE(2)

RGT K 7732-18-5 Water
 SOL 7732-18-5 Water

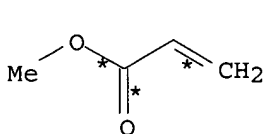
PRO BC 501419-34-7

RX(476) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20),
 RX(5), RX(9), RX(24), RX(10), RX(25), RX(26), RX(29), RX(30), RX(31),
 RX(11)

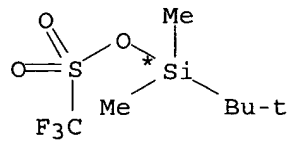
RX(476) U + V + 3 BY + CF + 2 BD + AT + CV + 2 CX ==>
BE



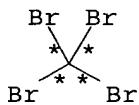
U



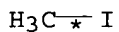
V



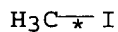
3 BY



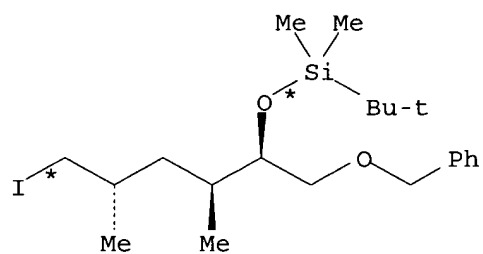
CF



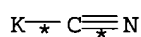
BD



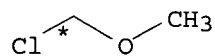
BD



AT

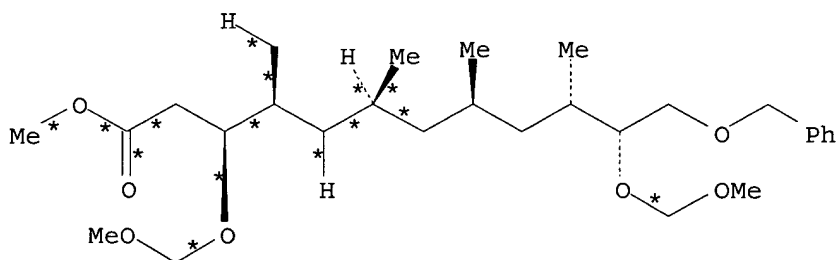


CV



2 CX

16
STEPS
→



BE
YIELD 88%

RX (4)

STAGE (1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, 12112-67-3
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE (2)

RGT X 760-32-7 MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)

RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RCT BY 69739-34-0
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)2
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)

RGT O 67-56-1 MeOH

STAGE(3)

RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH2Cl2

CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)

RGT AI 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)

RCT CD 501419-21-2

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) -78 deg C

SUBSTAGE(2) 30 minutes, -78 deg C

SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

RX(20) RCT CG 501419-22-3

STAGE(1)

RGT CH 109-72-8 BuLi

SOL 109-99-9 THF, 110-54-3 Hexane

CON SUBSTAGE(1) -78 deg C

SUBSTAGE(2) -78 deg C -> -25 deg C

SUBSTAGE(3) 1 hour, -25 deg C

SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)

RCT BD 74-88-4

SOL 109-99-9 THF

CON SUBSTAGE(1) -78 deg C

SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)

RGT AQ 12125-02-9 NH4Cl

SOL 7732-18-5 Water

PRO AB 501419-23-4

RX(5) RCT AB 501419-23-4

STAGE(1)

RGT AD 37342-97-5 Hydrozirconocene Cl

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 2 hours, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RGT AE 7553-56-2 I2

SOL 56-23-5 CCl4

CON 0 deg C

PRO AC 501419-02-9

NTE in the dark, regioselective, stereoselective

RX(9) RCT AT 501419-06-3

STAGE(1)

RGT AV 7646-85-7 ZnCl₂
SOL 60-29-7 Et₂O
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C

STAGE(2)

RGT AW 594-19-4 t-BuLi
SOL 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 5 minutes, -78 deg C
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RCT AC 501419-02-9
CAT 14221-01-3 Pd(PPh₃)₄
CON 16 hours, room temperature

STAGE(4)

RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO AU 501419-08-5
NTE modified Negishi coupling, stage three in the dark

RX(24) RCT AU 501419-08-5
RGT CM 429-41-4 Bu₄N.F
PRO AY 501419-27-8
SOL 109-99-9 THF
CON 20 hours, room temperature
NTE mol. sieves

RX(10) RCT AY 501419-27-8
RGT BA 1333-74-0 H₂
PRO AZ 501419-10-9
CAT 82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,4-butanediylbis[diphenylphosphine-κP]]-, tetrafluoroborate(1-)
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 4 hours, room temperature, 700 psi
NTE high pressure, stereoselective

RX(25) RCT AZ 501419-10-9, BY 69739-34-0

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature -> 0 deg C
SUBSTAGE(2) 5 minutes, 0 deg C
SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

STAGE(2)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO CN 501419-28-9

RX(26) RCT CN 501419-28-9

STAGE(1)

RGT CP 84-58-2 DDQ
SOL 75-09-2 CH₂Cl₂, 7732-18-5 Water
CON 1 hour, room temperature, pH 7

STAGE(2)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO CO 501419-29-0
NTE chemoselective, buffered soln.

RX(29) RCT CO 501419-29-0

STAGE(1)

RGT CQ 124-63-0 MeSO₂Cl, D 121-44-8 Et₃N
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C
SUBSTAGE(3) 3 minutes, 0 deg C
SUBSTAGE(4) 1.5 hours, 0 deg C -> room temperature

STAGE(2)

RGT K 7732-18-5 Water

STAGE(3)

RGT CT 7664-39-3 HF
SOL 75-05-8 MeCN, 7732-18-5 Water
CON 3 hours, room temperature

STAGE(4)

RGT BJ 584-08-7 K₂CO₃
SOL 67-56-1 MeOH
CON 45 minutes, room temperature

PRO CU 501419-32-5

RX(30) RCT CU 501419-32-5, CV 151-50-8
PRO CW 501419-33-6
SOL 75-05-8 MeCN
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 70 deg C
SUBSTAGE(3) 24 hours, 70 deg C
SUBSTAGE(4) 70 deg C -> room temperature

RX(31) RCT CW 501419-33-6, CX 107-30-2

STAGE(1)

RGT CY 7087-68-5 EtN(Pr-i)₂
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 28 hours, 0 deg C -> room temperature

STAGE(2)

RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO BC 501419-34-7

RX(11) RCT BC 501419-34-7

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)₂
 SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
 CON 1 hour, -78 deg C

STAGE(2)

RGT N 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON SUBSTAGE(2) 20 minutes, room temperature

STAGE(3)

RGT BG 513-35-9 Me₂C:CHMe, BH 7758-19-2 NaOClO, BI 7558-80-7
 NaH₂PO₄
 SOL 75-65-0 t-BuOH, 7732-18-5 Water
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 1 hour, 0 deg C

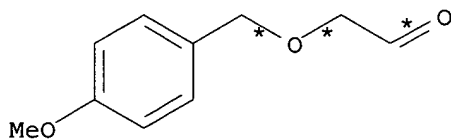
STAGE(4)

RCT BD 74-88-4
 RGT BJ 584-08-7 K₂CO₃
 SOL 68-12-2 DMF
 CON 3.5 hours, room temperature

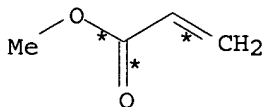
PRO BE 501419-14-3

RX(477) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20),
 RX(5), RX(9), RX(24), RX(10), RX(25), RX(26), RX(29), RX(30), RX(31),
 RX(32)

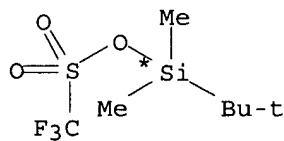
RX(477) U + V + 3 BY + CF + BD + AT + CV + 2 CX ==>
 CZ



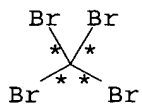
U



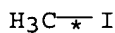
V



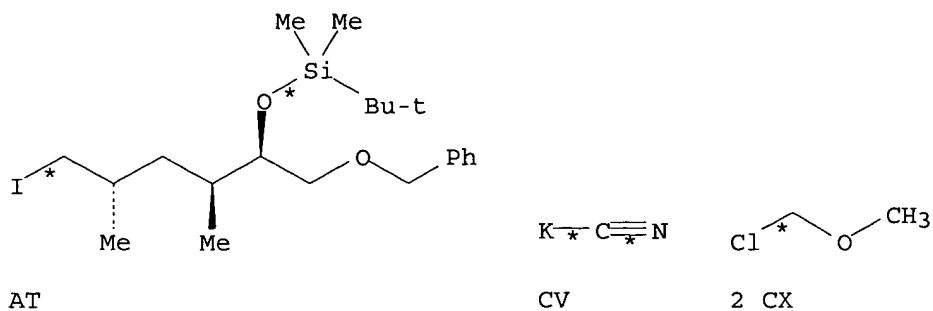
3 BY



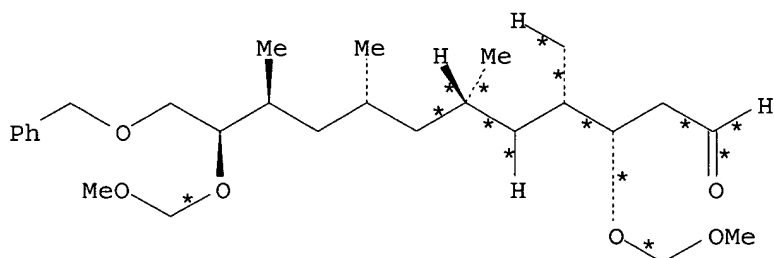
CF



BD



16
STEPS
→



RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]]-, 12112-67-3
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH₂CH₂Cl
CON 1 hour, room temperature

STAGE(2)

RGT X 760-32-7 MeEt₂SiH
SOL 107-06-2 ClCH₂CH₂Cl
CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH₂CH₂Cl
CON 48 hours, room temperature

STAGE(4)

RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)₂
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)

RGT O 67-56-1 MeOH

STAGE(3)

RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)

RGT AI 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)

RCT CD 501419-21-2
SOL 75-09-2 CH₂Cl₂

CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 30 minutes, -78 deg C
SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

RX(20) RCT CG 501419-22-3

STAGE(1)

RGT CH 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -25 deg C
SUBSTAGE(3) 1 hour, -25 deg C
SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)

RCT BD 74-88-4
SOL 109-99-9 THF
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)

RGT AQ 12125-02-9 NH4Cl
SOL 7732-18-5 Water

PRO AB 501419-23-4

RX(5) RCT AB 501419-23-4

STAGE(1)

RGT AD 37342-97-5 Hydrozirconocene Cl
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 2 hours, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RGT AE 7553-56-2 I2
SOL 56-23-5 CCl4
CON 0 deg C

PRO AC 501419-02-9

NTE in the dark, regioselective, stereoselective

RX(9) RCT AT 501419-06-3

STAGE(1)

RGT AV 7646-85-7 ZnCl2
SOL 60-29-7 Et2O
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C

STAGE(2)

RGT AW 594-19-4 t-BuLi
SOL 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 5 minutes, -78 deg C
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RCT AC 501419-02-9
CAT 14221-01-3 Pd(PPh₃)₄
CON 16 hours, room temperature

STAGE(4)

RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO AU 501419-08-5
NTE modified Negishi coupling, stage three in the dark

RX(24) RCT AU 501419-08-5
RGT CM 429-41-4 Bu₄N.F
PRO AY 501419-27-8
SOL 109-99-9 THF
CON 20 hours, room temperature
NTE mol. sieves

RX(10) RCT AY 501419-27-8
RGT BA 1333-74-0 H₂
PRO AZ 501419-10-9
CAT 82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,4-butanediylbis[diphenylphosphine-κP]]-, tetrafluoroborate(1-)
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 4 hours, room temperature, 700 psi
NTE high pressure, stereoselective

RX(25) RCT AZ 501419-10-9, BY 69739-34-0

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature -> 0 deg C
SUBSTAGE(2) 5 minutes, 0 deg C
SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

STAGE(2)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO CN 501419-28-9

RX(26) RCT CN 501419-28-9

STAGE(1)

RGT CP 84-58-2 DDQ
SOL 75-09-2 CH₂Cl₂, 7732-18-5 Water
CON 1 hour, room temperature, pH 7

STAGE(2)

RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO CO 501419-29-0
NTE chemoselective, buffered soln.

RX(29) RCT CO 501419-29-0

STAGE(1)

RGT CQ 124-63-0 MeSO₂Cl, D 121-44-8 Et₃N
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C
SUBSTAGE(3) 3 minutes, 0 deg C
SUBSTAGE(4) 1.5 hours, 0 deg C -> room temperature

STAGE(2)

RGT K 7732-18-5 Water

STAGE(3)

RGT CT 7664-39-3 HF
SOL 75-05-8 MeCN, 7732-18-5 Water
CON 3 hours, room temperature

STAGE(4)

RGT BJ 584-08-7 K₂CO₃
SOL 67-56-1 MeOH
CON 45 minutes, room temperature

PRO CU 501419-32-5

RX(30) RCT CU 501419-32-5, CV 151-50-8
PRO CW 501419-33-6
SOL 75-05-8 MeCN
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 70 deg C
SUBSTAGE(3) 24 hours, 70 deg C
SUBSTAGE(4) 70 deg C -> room temperature

RX(31) RCT CW 501419-33-6, CX 107-30-2

STAGE(1)

RGT CY 7087-68-5 EtN(Pr-i)₂
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 28 hours, 0 deg C -> room temperature

STAGE(2)

RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO BC 501419-34-7

RX(32) RCT BC 501419-34-7

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)₂
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON 1 hour, -78 deg C

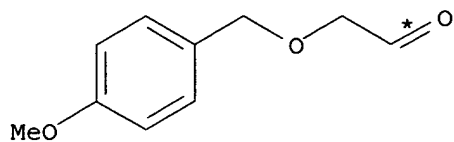
STAGE(2)

RGT N 7647-01-0 HCl
SOL 7732-18-5 Water
CON SUBSTAGE(2) 20 minutes, room temperature

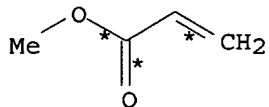
PRO CZ 501419-35-8

RX(555) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20),
RX(5), RX(9), RX(24), RX(10)

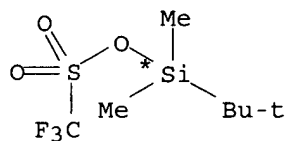
RX(555) U + V + BY + CF + BD + AT ==> AZ



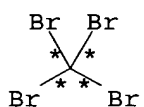
U



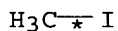
V



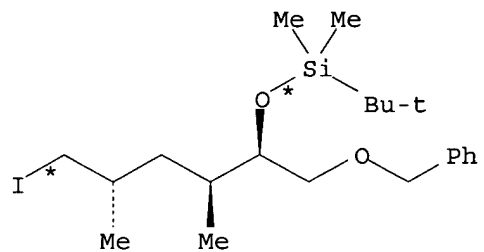
BY



CF

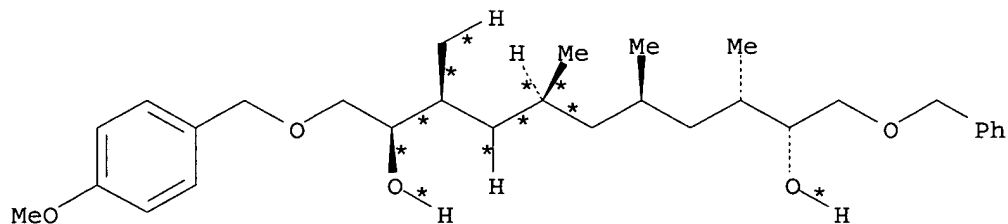


BD



AT

10
STEPS
→



AZ

YIELD 86%

RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, 12112-67-3

Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-

SOL 107-06-2 ClCH₂CH₂Cl

CON 1 hour, room temperature

STAGE(2)

RGT X 760-32-7 MeEt₂SiH

SOL 107-06-2 ClCH₂CH₂Cl

CON 30 minutes, room temperature

STAGE(3)

RCT U 121289-23-4, V 96-33-3

SOL 107-06-2 ClCH₂CH₂Cl

CON 48 hours, room temperature

STAGE(4)

RGT N 7647-01-0 HCl

SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water

CON 30 minutes, room temperature

PRO W 501419-01-8

NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine

SOL 75-09-2 CH₂Cl₂

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)

RCT BY 69739-34-0

SOL 75-09-2 CH₂Cl₂

CON SUBSTAGE(1) 15 minutes, 0 deg C

SUBSTAGE(2) 0 deg C -> room temperature

SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT G 144-55-8 NaHCO₃

SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)

RGT BF 1191-15-7 AlH(Bu-i)₂

SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane

CON SUBSTAGE(1) -78 deg C

SUBSTAGE(2) 45 minutes, -78 deg C

SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)

RGT O 67-56-1 MeOH

STAGE(3)

RGT CC 304-59-6 Rochelle salt

SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)
RGT AI 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)
RCT CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 30 minutes, -78 deg C
SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

RX(20) RCT CG 501419-22-3

STAGE(1)
RGT CH 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -25 deg C
SUBSTAGE(3) 1 hour, -25 deg C
SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)
RCT BD 74-88-4
SOL 109-99-9 THF
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)
RGT AQ 12125-02-9 NH₄Cl
SOL 7732-18-5 Water

PRO AB 501419-23-4

RX(5) RCT AB 501419-23-4

STAGE(1)
RGT AD 37342-97-5 Hydrozirconocene Cl
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 2 hours, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RGT AE 7553-56-2 I₂
SOL 56-23-5 CCl₄
CON 0 deg C

PRO AC 501419-02-9
NTE in the dark, regioselective, stereoselective

RX(9) RCT AT 501419-06-3

STAGE(1)

RGT AV 7646-85-7 ZnCl₂
SOL 60-29-7 Et₂O
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C

STAGE(2)

RGT AW 594-19-4 t-BuLi
SOL 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 5 minutes, -78 deg C
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RCT AC 501419-02-9
CAT 14221-01-3 Pd(PPh₃)₄
CON 16 hours, room temperature

STAGE(4)

RGT K 7732-18-5 Water
SOL 7732-18-5 Water

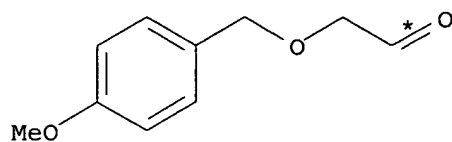
PRO AU 501419-08-5
NTE modified Negishi coupling, stage three in the dark

RX(24) RCT AU 501419-08-5
RGT CM 429-41-4 Bu₄N.F
PRO AY 501419-27-8
SOL 109-99-9 THF
CON 20 hours, room temperature
NTE mol. sieves

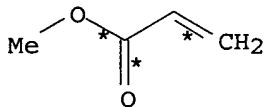
RX(10) RCT AY 501419-27-8
RGT BA 1333-74-0 H₂
PRO AZ **501419-10-9**
CAT 82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene] [1,4-butanediylbis[diphenylphosphine-κP]]-, tetrafluoroborate(1-)
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 4 hours, room temperature, 700 psi
NTE high pressure, stereoselective

RX(558) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20),
RX(5), RX(9), RX(24), RX(10), RX(25)

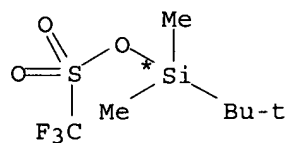
RX(558) U + V + 3 BY + CF + BD + AT ==> **CN**



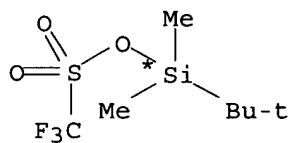
U



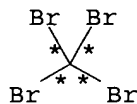
V



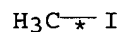
BY



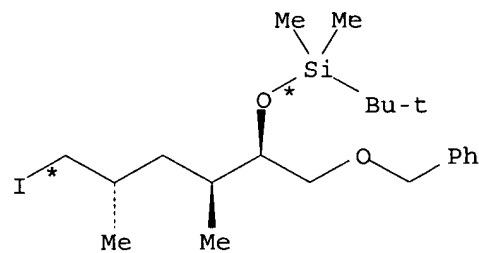
2 BY



CF

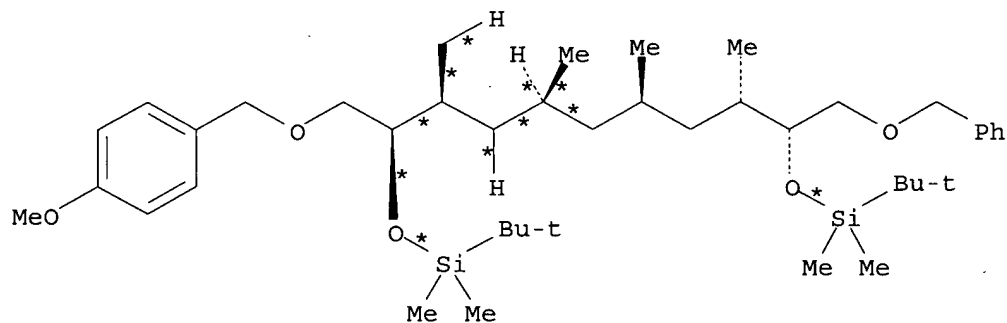


BD



AT

11
STEPS
→



CN

YIELD 100%

RX(4)

STAGE(1)

CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-

[2(3aR*,8aS*),3a α ,8a α]]-, 12112-67-3
Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-
cyclooctadiene]di-
SOL 107-06-2 ClCH₂CH₂Cl
CON 1 hour, room temperature

STAGE(2)
RGT X 760-32-7 MeEt₂SiH
SOL 107-06-2 ClCH₂CH₂Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH₂CH₂Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RGT G 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)
RGT BF 1191-15-7 AlH(Bu-i)₂
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)
RGT O 67-56-1 MeOH

STAGE(3)
RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON 90 minutes, room temperature

RX(19) RCT CF 558-13-4

STAGE(1)
RGT AI 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> -78 deg C

STAGE(2)
RCT CD 501419-21-2
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 30 minutes, -78 deg C
SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG 501419-22-3

RX(20) RCT CG 501419-22-3

STAGE(1)
RGT CH 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -25 deg C
SUBSTAGE(3) 1 hour, -25 deg C
SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)
RCT BD 74-88-4
SOL 109-99-9 THF
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)
RGT AQ 12125-02-9 NH₄Cl
SOL 7732-18-5 Water

PRO AB 501419-23-4

RX(5) RCT AB 501419-23-4

STAGE(1)
RGT AD 37342-97-5 Hydrozirconocene Cl
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 2 hours, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RGT AE 7553-56-2 I₂
SOL 56-23-5 CCl₄
CON 0 deg C

PRO AC 501419-02-9
NTE in the dark, regioselective, stereoselective

RX(9) RCT AT 501419-06-3

STAGE(1)

RGT AV 7646-85-7 ZnCl₂
SOL 60-29-7 Et₂O
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C

STAGE(2)

RGT AW 594-19-4 t-BuLi
SOL 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 5 minutes, -78 deg C
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RCT AC 501419-02-9
CAT 14221-01-3 Pd(PPh₃)₄
CON 16 hours, room temperature

STAGE(4)

RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO AU 501419-08-5
NTE modified Negishi coupling, stage three in the dark

RX(24) RCT AU 501419-08-5
RGT CM 429-41-4 Bu₄N.F
PRO AY 501419-27-8
SOL 109-99-9 THF
CON 20 hours, room temperature
NTE mol. sieves

RX(10) RCT AY 501419-27-8
RGT BA 1333-74-0 H₂
PRO AZ 501419-10-9
CAT 82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene] [1,4-butanediylbis[diphenylphosphine-κP]]-, tetrafluoroborate(1-)
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 4 hours, room temperature, 700 psi
NTE high pressure, stereoselective

RX(25) RCT AZ 501419-10-9, BY 69739-34-0

STAGE(1)

RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) room temperature -> 0 deg C
SUBSTAGE(2) 5 minutes, 0 deg C
SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

STAGE(2)

RGT G 144-55-8 NaHCO₃

SOL 7732-18-5 Water

PRO CN 501419-28-9

L64 ANSWER 19 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 137:185334 CASREACT

TITLE: Stereoselective Synthesis of trans β -Lactams
through Iridium-Catalyzed Reductive Coupling of Imines
and Acrylates

AUTHOR(S) : Townes, Jennifer A.; Evans, Michael A.; Queffelec, Jerome; Taylor, Steven J.; Morken, James P.

CORPORATE SOURCE: Department of Chemistry, Venable and Kenan
Laboratories, University of North Carolina at Chapel
Hill, Chapel Hill, NC, 27599-3290, USA

SOURCE: Organic Letters (2002), 4(15), 2537-2540

CODEN: ORLEF7; ISSN: 1523-7060

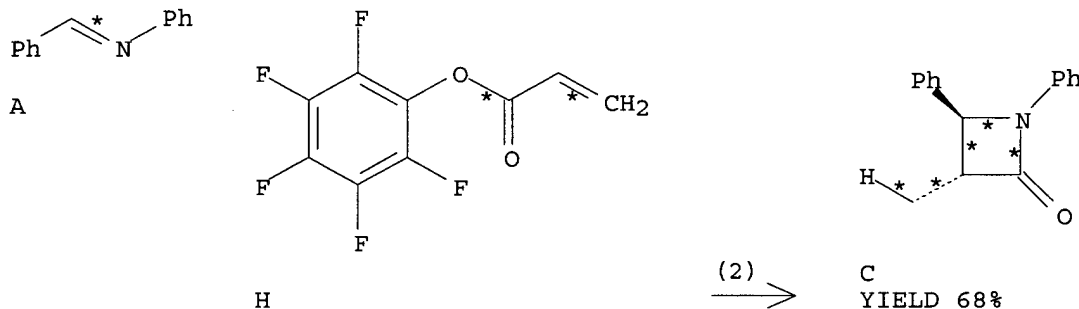
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Iridium-catalyzed reductive coupling of acrylates and imines provides trans β -lactams with high diastereoselection. The optimal catalyst allows for the synthesis of trans β -lactams bearing aromatic, alkenyl, and alkynyl side chains. This reaction appears to proceed through a reductive Mannich addition-cyclization mechanism. Examination of substituent effects reveals a linear Hammett correlation for both the N-aryl group on the imine and the aryloxy group on the acrylate, thereby pointing to rate-determining cyclization in the reaction mechanism.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

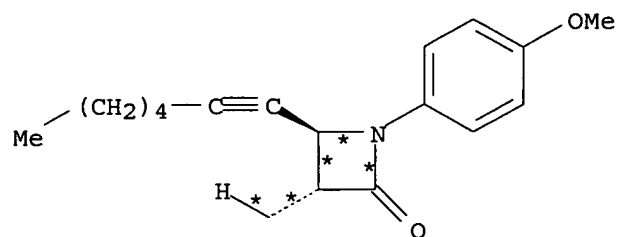
$$\text{RX (2) OF 8} \quad \text{A} + \text{H} \implies \text{C}$$


```

RX(2)      RCT  A 538-51-2, H 71195-85-2
           RGT  D 760-32-7 MeEt2SiH
           PRO  C 17324-17-3
           CAT  12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-
           1,5-cyclooctadiene]di-, 101-02-0 P(OPh)3
           SOL  107-06-2 ClCH2CH2Cl
           NTE  stereoselective, optimization study, optimized on metal
           catalyst/liqand/silane

```

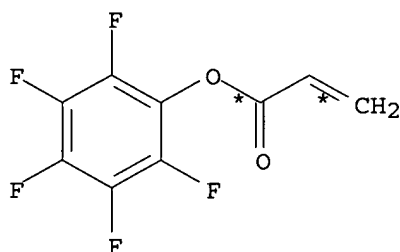
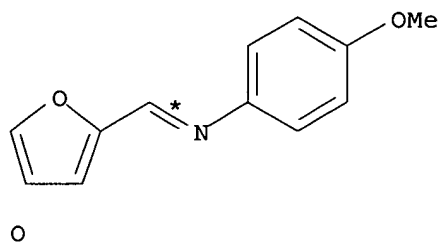
$$RX(3) \text{ OF } 8 \quad K + H \implies L$$



N
YIELD 58%

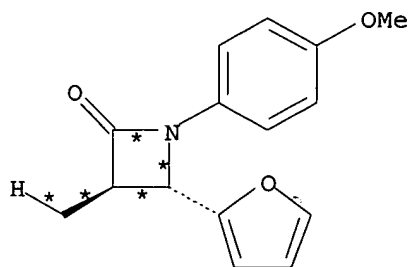
RX(4) RCT M 451455-39-3, H 71195-85-2
 RGT D 760-32-7 MeEt2SiH
 PRO N 451455-42-8
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η) -
 1,5-cyclooctadiene]di-, 101-02-0 P(OPh)3
 SOL 107-06-2 ClCH2CH2Cl
 NTE stereoselective

RX(5) OF 8 O + H ==> P



H

(5) →

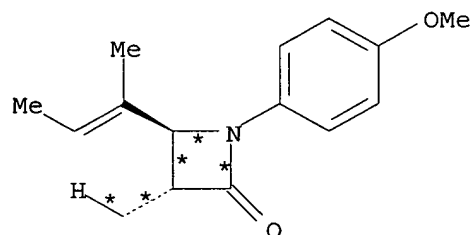
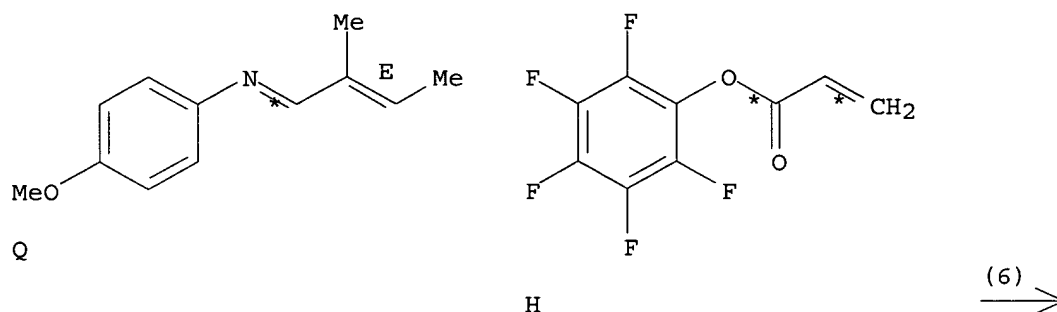


P
YIELD 78%

RX(5) RCT O 1749-14-0, H 71195-85-2
 RGT D 760-32-7 MeEt2SiH

PRO P 152899-73-5
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-
 1,5-cyclooctadiene]di-, 101-02-0 P(OPh)₃
 SOL 107-06-2 ClCH₂CH₂Cl
 NTE stereoselective

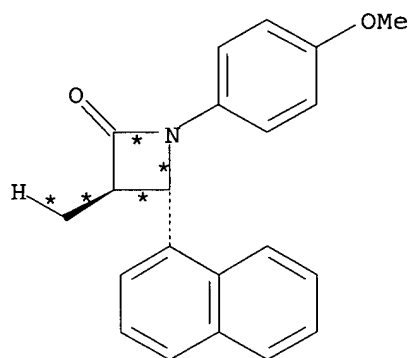
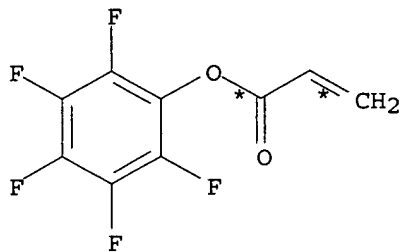
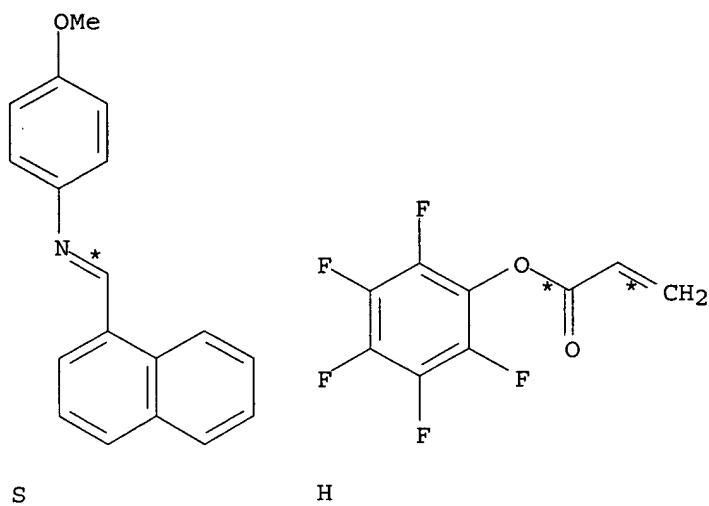
RX(6) OF 8 Q + H ==> R



YIELD 60%

RX(6) RCT Q 451455-40-6, H 71195-85-2
 RGT D 760-32-7 MeEt₂SiH
 PRO R 451455-43-9
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-
 1,5-cyclooctadiene]di-, 101-02-0 P(OPh)₃
 SOL 107-06-2 ClCH₂CH₂Cl
 NTE stereoselective

RX(7) OF 8 S + H ==> T



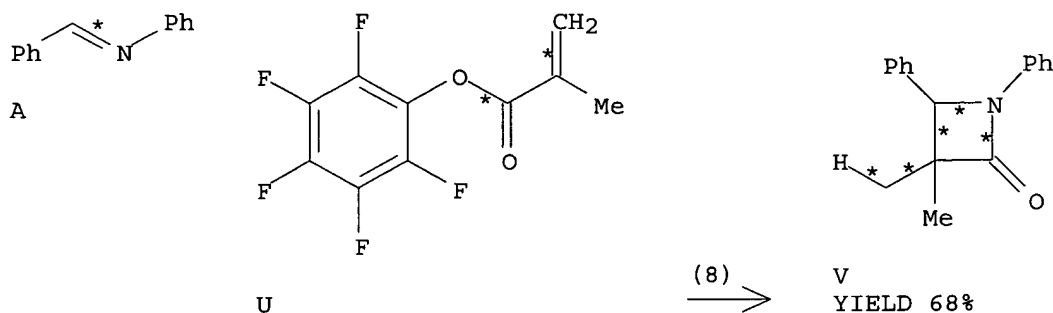
T
YIELD 80%

```

RX(7)      RCT  S 3525-60-8, H 71195-85-2
           RGT  D 760-32-7 MeEt2SiH
           PRO  T 451455-44-0
           CAT  12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-
           1,5-cyclooctadiene]di-, 101-02-0 P(OPh)3
           SOL  107-06-2 ClCH2CH2Cl
           NTE  stereoselective

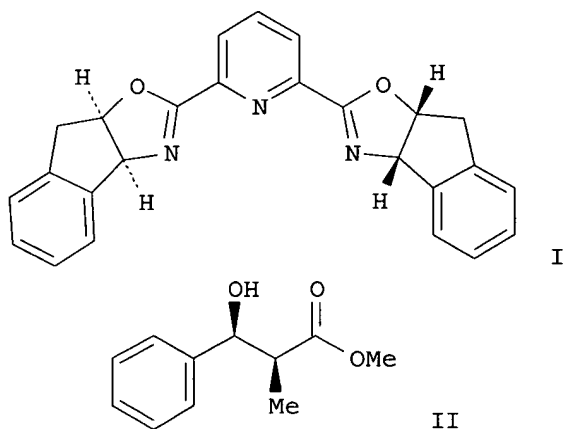
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$$RX(8) \quad OF \quad 8 \quad A + U ==> V$$



RX(8) RCT A 538-51-2, U 13642-97-2
RGT D 760-32-7 MeEt2SiH
PRO V 5438-81-3
CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-
1,5-cyclooctadiene]di-, 101-02-0 P(OPh)3
SOL 107-06-2 ClCH2CH2Cl

L64 ANSWER 20 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 135:107055 CASREACT
TITLE: Enantio- and diastereoselective reductive aldol
reactions with iridium-pybox catalysts
AUTHOR(S): Zhao, Cun-Xiang; Duffey, Matthew O.; Taylor, Steven
J.; Morken, James P.
CORPORATE SOURCE: Department of Chemistry Venable and Kenan
Laboratories, The University of North Carolina at
Chapel Hill, Chapel Hill, NC, 27599-3290, USA
SOURCE: Organic Letters (2001), 3(12), 1829-1831
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

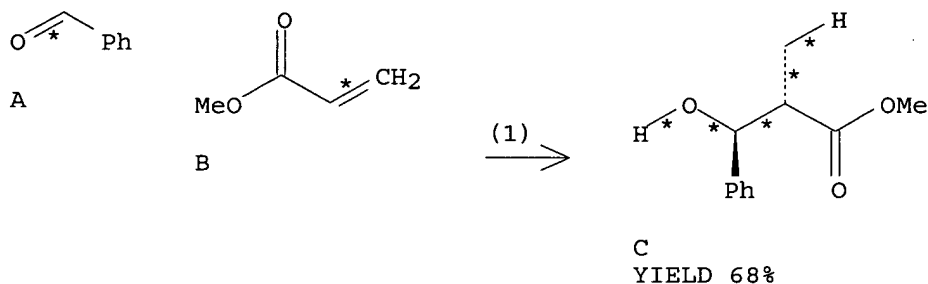


AB A catalytic amount of [(COD)IrCl]₂ and indane-pybox I converts diethylmethyilsilane, Me acrylate, and certain aldehydes to the derived

reductive aldol adduct with good enantio- and diastereocontrol. Thus, reaction of PhCHO with H₂C:CHCO₂Me and Et₂SiHMe in CH₂Cl₂ containing [(COD)IrCl]₂ and I at 25° for 24 h gave the hydroxybenzenepropanoate II in 68% yield with 6.6:1 syn:anti ratio and 97:3 enantiomeric ratio.

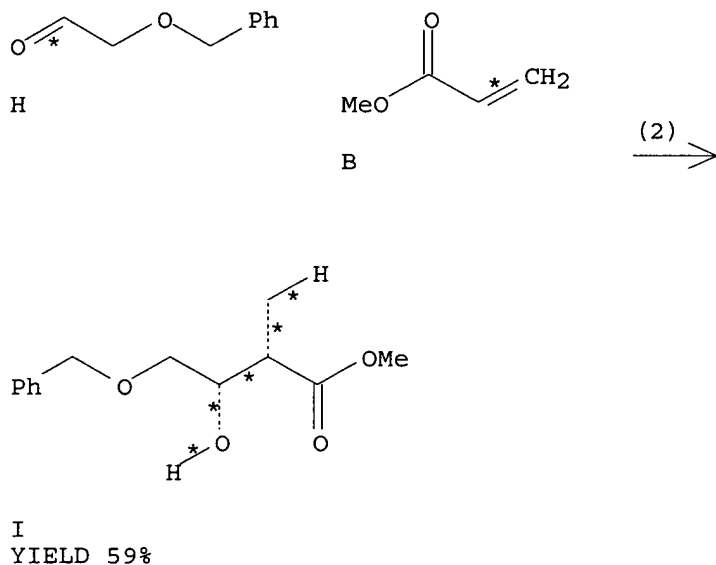
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 7 A + B ==> C



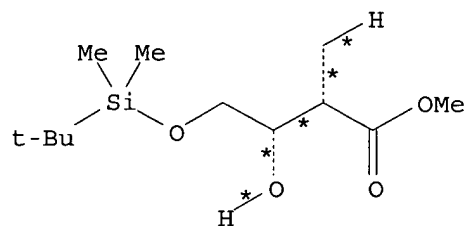
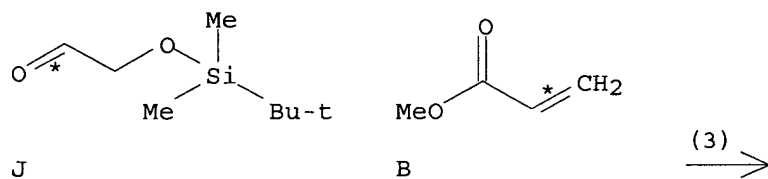
RX(1) RCT A 100-52-7, B 96-33-3
 RGT D 760-32-7 MeEt₂SiH
 PRO C 76549-03-6
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]]-
 SOL 75-09-2 CH₂Cl₂
 NTE stereoselective

RX(2) OF 7 H + B ==> I



RX(2) RCT H 60656-87-3, B 96-33-3
 RGT D 760-32-7 MeEt2SiH
 PRO I 350256-93-8
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-
 1,5-cyclooctadiene]di-, 185346-09-2 8H-Indeno[1,2-d]oxazole,
 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-
 [2(3aR*,8aS*),3aα,8aα]]-
 SOL 75-09-2 CH2Cl2
 NTE stereoselective

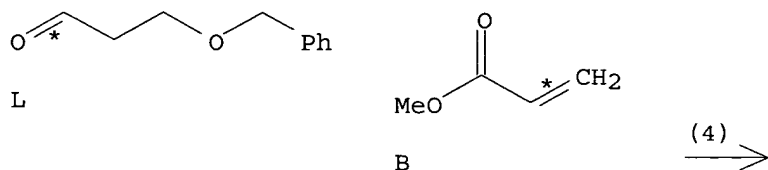
RX(3) OF 7 J + B ==> K

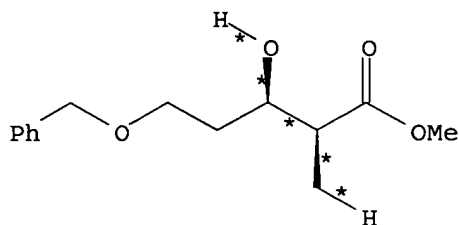


K
 YIELD 47%

RX(3) RCT J 102191-92-4, B 96-33-3
 RGT D 760-32-7 MeEt2SiH
 PRO K 350256-94-9
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-
 1,5-cyclooctadiene]di-, 185346-09-2 8H-Indeno[1,2-d]oxazole,
 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-
 [2(3aR*,8aS*),3aα,8aα]]-
 SOL 75-09-2 CH2Cl2
 NTE stereoselective

RX(4) OF 7 L + B ==> M

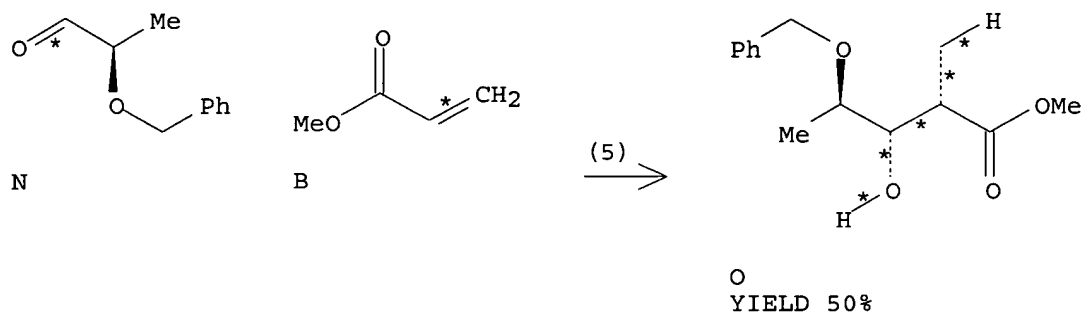




M
YIELD 65%

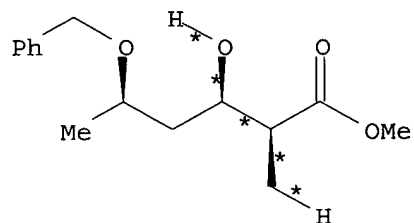
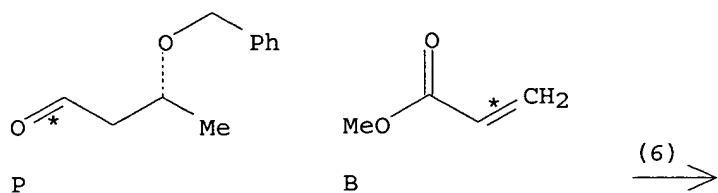
RX(4) RCT L 19790-60-4, B 96-33-3
 RGT D 760-32-7 MeEt₂SiH
 PRO M 350256-95-0
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-
 1,5-cyclooctadiene]di-, 185346-09-2 8H-Indeno[1,2-d]oxazole,
 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-
 [2(3aR*,8aS*),3aα,8aα]]-
 SOL 75-09-2 CH₂Cl₂
 NTE stereoselective

RX(5) OF 7 N + B ==> O



RX(5) RCT N 81445-45-6, B 96-33-3
 RGT D 760-32-7 MeEt₂SiH
 PRO O 350256-96-1
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-
 1,5-cyclooctadiene]di-, 185346-09-2 8H-Indeno[1,2-d]oxazole,
 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-
 [2(3aR*,8aS*),3aα,8aα]]-
 SOL 75-09-2 CH₂Cl₂
 NTE stereoselective

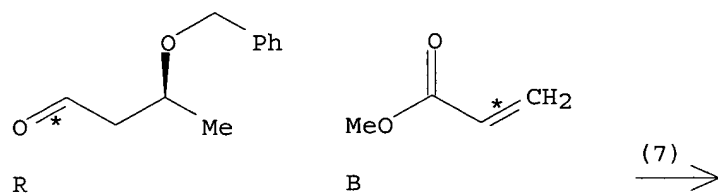
RX(6) OF 7 P + B ==> Q

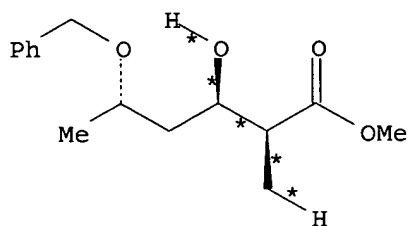


Q
YIELD 65%

RX(6) RCT P 86040-07-5, B 96-33-3
 RGT D 760-32-7 MeEt2SiH
 PRO Q 350256-97-2
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-
 1,5-cyclooctadiene]di-, 185346-09-2 8H-Indeno[1,2-d]oxazole,
 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-
 [2(3aR*,8aS*),3aα,8aα]]-
 SOL 75-09-2 CH2Cl2
 NTE stereoselective

RX(7) OF 7 R + B ==> S

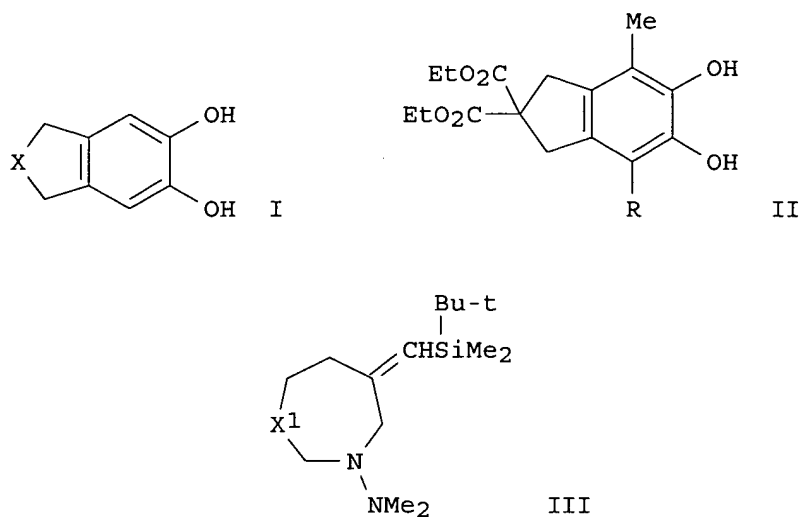




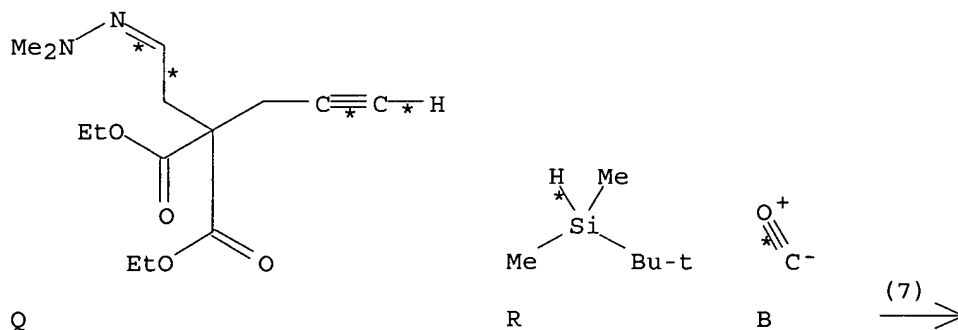
S
YIELD 57%

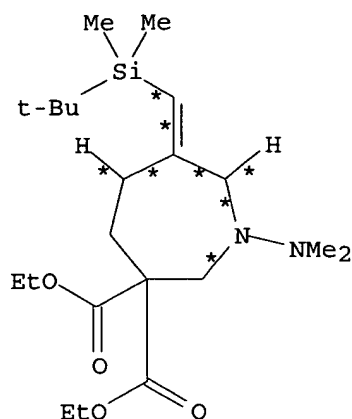
RX(7) RCT R 99032-03-8, B 96-33-3
RGT D 760-32-7 MeEt2SiH
PRO S 350256-98-3
CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-
1,5-cyclooctadiene]di-, 185346-09-2 8H-Indeno[1,2-d]oxazole,
2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-
[2(3aR*,8aS*),3a α ,8a α]]-
SOL 75-09-2 CH2Cl2
NTE stereoselective

L64 ANSWER 21 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 129:67445 CASREACT
TITLE: Development of novel catalytic systems based on
transition metal complexes
AUTHOR(S): Murai, Shinji
CORPORATE SOURCE: Japan
SOURCE: Asahi Garasu Zaidan Josei Kenkyu Seika Hokoku
[Electronic Publication] (1996) No pp. Given
CODEN: AGSHEN; ISSN: 0919-9179
PUBLISHER: Asahi Garasu Zaidan
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: Japanese
GI



AB The reaction of 1,6-diynes HC.tplbond.CCH2XCH2C.tplbond.CH [X = C(CO2Et)2, CH2, O, NTs, S] or MeC.tplbond.CCH2C(CO2Et)2CH2C.tplbond.CR (R = H, Me) with H2O and CO (50 atm) in the presence of Ru3(CO)12 at 140°C in dioxane resulted in the incorporation of two mols. of CO to give catechol derivs. (I; X = same as above) or (II; R = H, Me) in good yields (58-83%). The reaction involves the intermediary of an oxycarbyne complex as a key catalytic species and is the new mode of successive incorporation of two mols. of CO into diynes. The reaction of acetylene-hydrazones HC.tplbond.CCH2X1CH2CH:NNMe2 [X1 = C(CO2Et)2, CH2, bond] with HSiMe2But and CO (10 atm) in the presence of Ir4(CO)12 at 140°C in CH3CN gave 6- or 7-membered nitrogen heterocycles (III; X1 = same as above) having a (trimethylsilyl)methylene group at 3-position. The reaction involves cyclization with incorporation of one mol. of CO and reduction of the incorporated CO carbon to methylene group. The reaction provides a new method for the construction of nitrogen heterocycles. Thus, reaction of HC.tplbond.CCH2C(CO2Et)2CH2C.tplbond.CH with H2O and CO in the presence of Ru3(CO)12 in dioxane at 50 atm and 140° gave 83% I [X = C(CO2Et)2].

$$\text{RX (7) OF 7} \quad \text{O} + \text{R} + \text{B} \implies \text{S}$$




S
YIELD 53%

RX(7) RCT Q 168557-46-8, R 29681-57-0, B 630-08-0
 PRO S 208830-57-3
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahydro
 SOL 75-05-8 MeCN
 NTE 10 atm and 140°

L64 ANSWER 22 OF 38 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 123:228275 CASREACT

TITLE: Iridium-Catalyzed Reaction of Acetylene Hydrazones
 with a Hydrosilane and Carbon Monoxide. Synthesis of
 Nitrogen Heterocycles

AUTHOR(S): Chatani, Naoto; Yamaguchi, Shinshi; Fukumoto, Yoshiya;
 Murai, Shinji

CORPORATE SOURCE: Faculty of Engineering, Osaka University, Suita, 565,
 Japan

SOURCE: Organometallics (1995), 14(9), 4418-20

CODEN: ORGND7; ISSN: 0276-7333

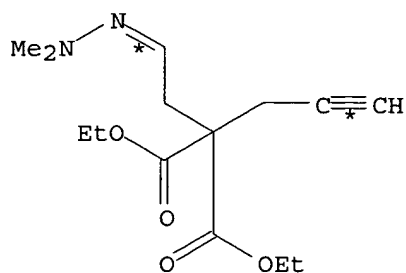
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

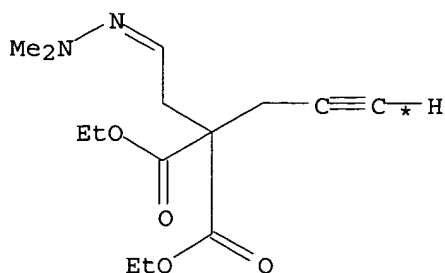
LANGUAGE: English

AB The reaction of acetylene hydrazones with a hydrosilane and carbon
 monoxide (CO) in the presence of Ir₄(CO)₁₂ as the catalyst gave six- or
 seven-membered nitrogen heterocycles having a (tert-
 butyldimethylsilyl)methylene group at the 3-position.

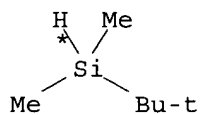
RX(2) OF 16 ...2 D + 2 F + G ==> H + I



D



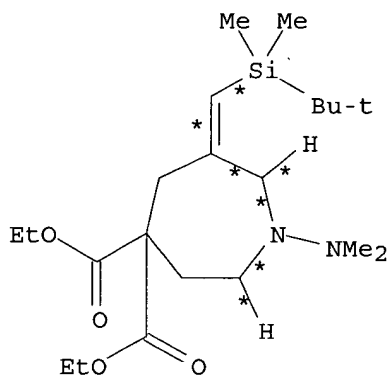
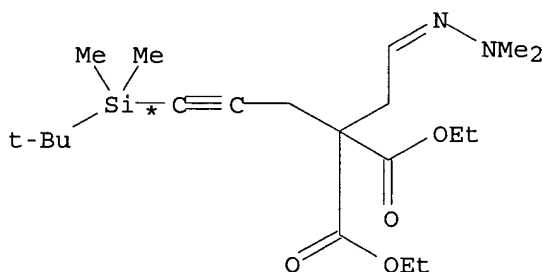
D



2 F

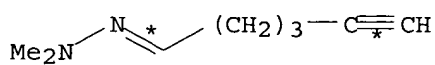


G

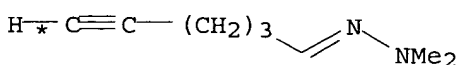
H
YIELD 53%I
YIELD 8%

RX(2) RCT D 168557-46-8, F 29681-57-0, G 630-08-0
 PRO H 168557-47-9, I 168557-48-0
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro
 SOL 75-05-8 MeCN
 NTE stereoselective, high pressure, optimization study, optimized on
 reaction temperature, pressure of CO, catalyst

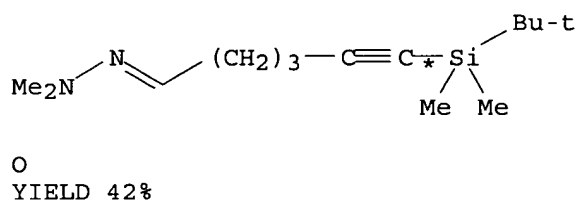
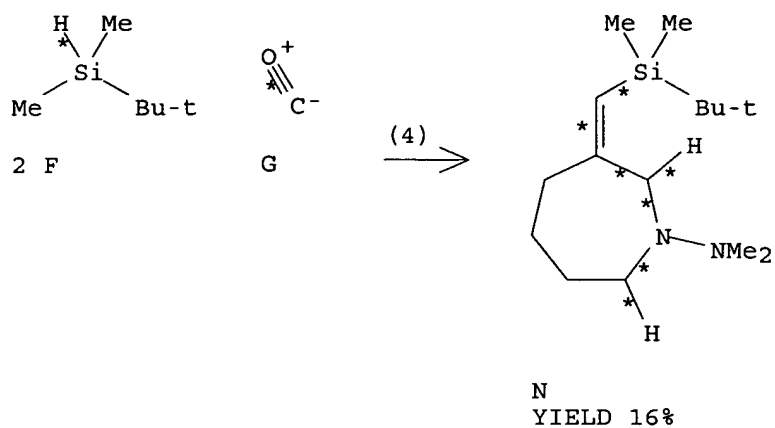
RX(4) OF 16 ... 2 M + 2 F + G ==> N + O



M

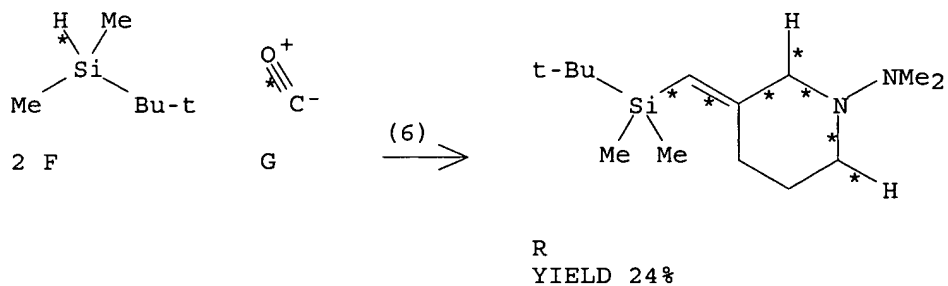
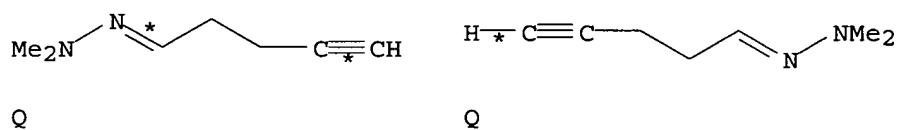


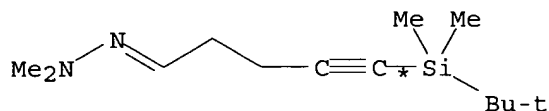
M



RX(4) RCT M 168557-50-4, F 29681-57-0, G 630-08-0
 PRO N 168557-51-5, O 168557-52-6
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro
 SOL 75-05-8 MeCN
 NTE stereoselective, high pressure

RX(6) OF 16 ... 2 Q + 2 F + G ==> R + S

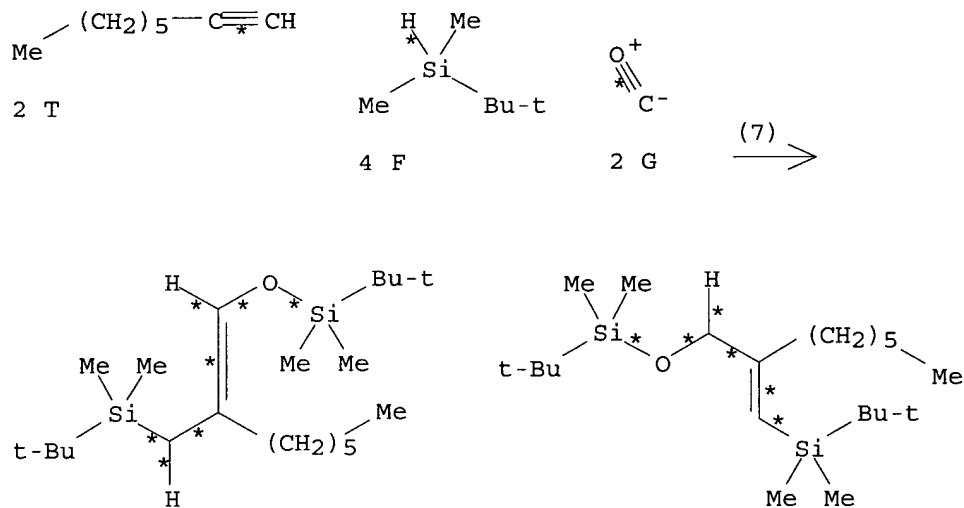




S
YIELD 24%

RX(6) RCT Q 168557-53-7, F 29681-57-0, G 630-08-0
 PRO R 168557-54-8, S 168557-55-9
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro
 SOL 75-05-8 MeCN
 NTE stereoselective, high pressure

RX(7) OF 16 2 T + 4 F + 2 G ==> U + V

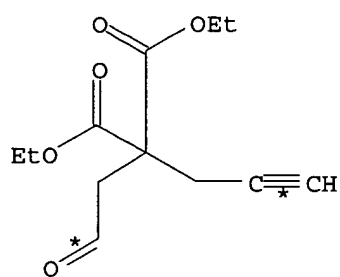


U
YIELD 20%

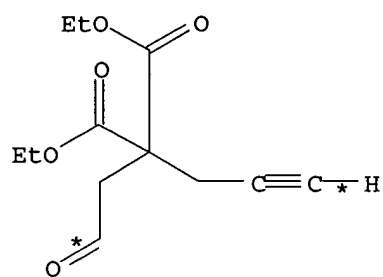
V
YIELD 7%

RX(7) RCT T 629-05-0, F 29681-57-0, G 630-08-0
 PRO U 168557-57-1, V 168557-56-0
 CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro
 SOL 75-05-8 MeCN
 NTE high pressure, other product(s) also detected

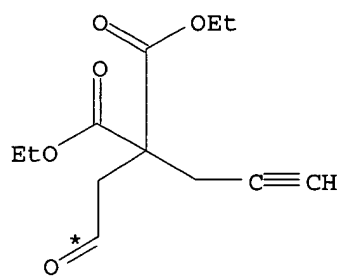
RX(11) OF 16 COMPOSED OF RX(1), RX(2)
 RX(11) 3 A + 2 B + 2 C + 2 F + G ==> H +
 I



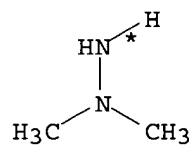
A



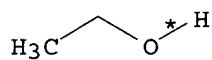
A



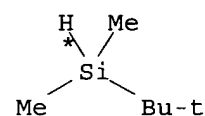
A



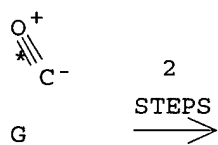
2 B



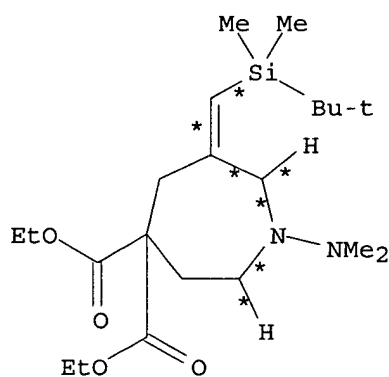
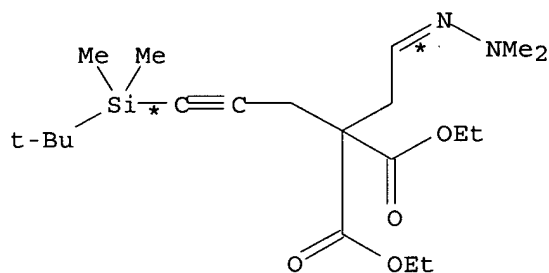
2 C



2 F

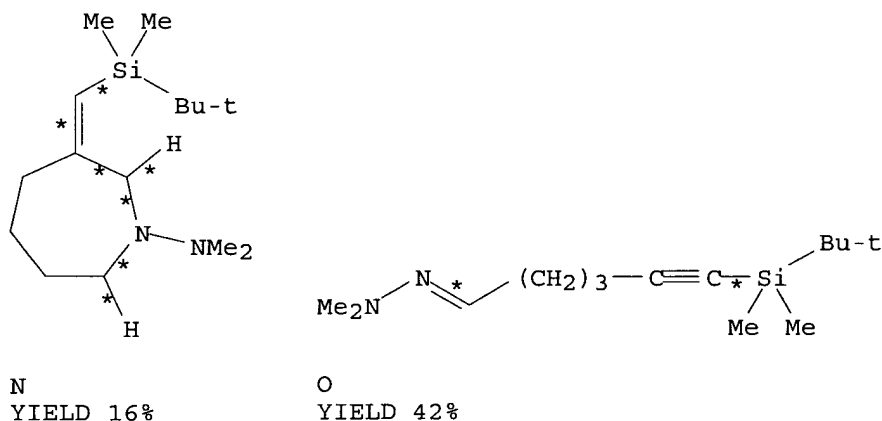
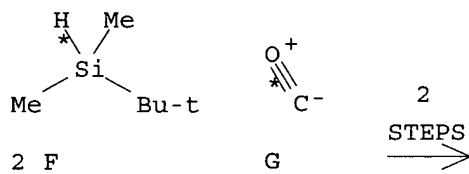
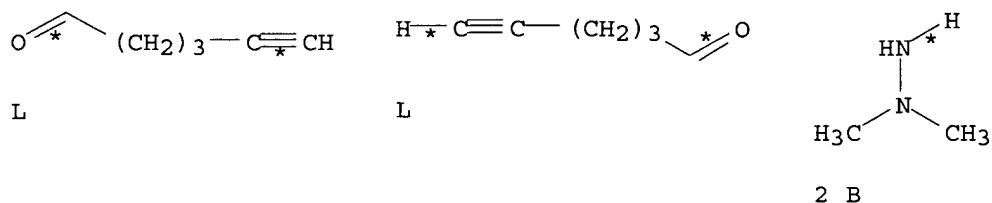


G

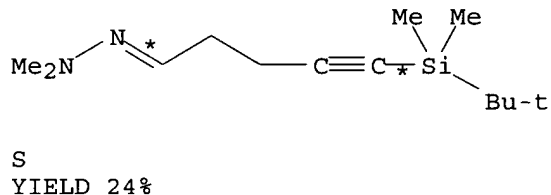
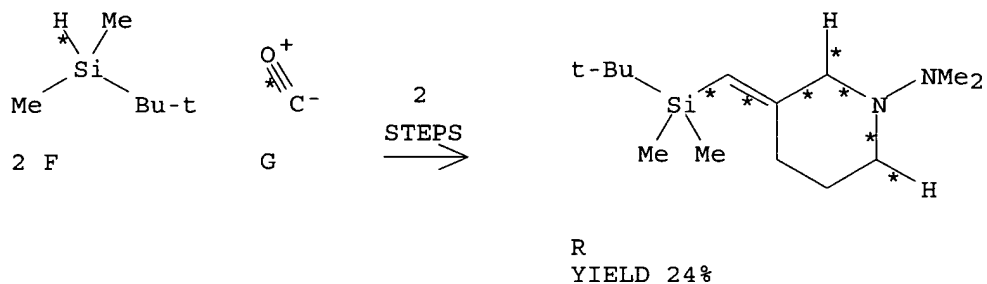
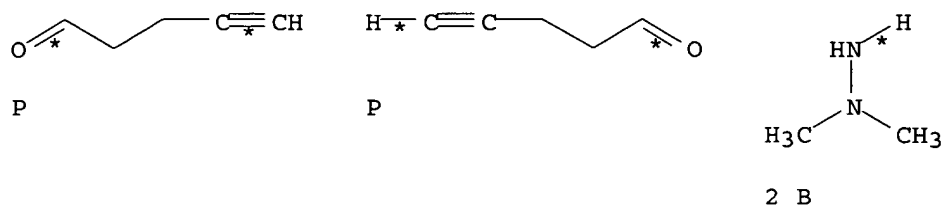
2
STEPS
→H
YIELD 53%I
YIELD 8%

RX(1) RCT A 137435-59-7, B 57-14-7, C 64-17-5

RX(2)	RCT	D 168557-46-8, F 29681-57-0, G 630-08-0
	PRO	H 168557-47-9, I 168557-48-0
	CAT	18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro
	SOL	75-05-8 MeCN
	NTE	stereoselective, high pressure, optimization study, optimized on reaction temperature, pressure of CO, catalyst

$$\text{RX (13)} \quad 2 \text{ L} + 2 \text{ B} + 2 \text{ F} + \text{G} \implies \text{N} + \text{O}$$


RX(4)	RCT	M 168557-50-4, F 29681-57-0, G 630-08-0
	PRO	N 168557-51-5, O 168557-52-6
	CAT	18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro
	SOL	75-05-8 MeCN
	NTE	stereoselective, high pressure

$$\text{RX (14)} \quad 2 \text{ P} + 2 \text{ B} + 2 \text{ F} + \text{G} \implies \text{R} + \text{S}$$


RX(6) RCT Q 168557-53-7, F 29681-57-0, G 630-08-0
PRO R 168557-54-8, S 168557-55-9
CAT 18827-81-1 Iridium, dodecacarbonyltetra-, tetrahedro
SOL 75-05-8 MeCN
NTE stereoselective, high pressure

L64 ANSWER 23 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:409220 HCAPLUS
DOCUMENT NUMBER: 144:412697
TITLE: Improved process for preparation of organosilanes by
hydrosilylation of **alkenes** in the presence
of iridium **diene** catalysts and oxidative
cocatalysts
INVENTOR(S): Baumann, Frank; Hofmann, Marco
PATENT ASSIGNEE(S): Wacker-Chemie G.m.b.H., Germany
SOURCE: PCT Int. Appl., 29 pp.

CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006045533	A1	20060504	WO 2005-EP11300	20051020
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
DE 102004052424	A1	20060504	DE 2004-102004052424	20041028
PRIORITY APPLN. INFO.: DE 2004-102004052424A 20041028 DE 2005-102005030581A 20050630				
AB	An improved process for preparation of alkylsilanes R ₆ R ₅ CHR ₄ CHSiR ₁ R ₂ R ₃ [R ₁ , R ₂ , R ₃ = C ₁ -18 alkyl(oxy), preferably R ₁ , R ₂ , R ₃ = (un)branched C ₁ -6 alkyl, C ₁ -6 alkoxy; R ₄ , R ₅ , R ₆ = H, organyl, optionally substituted by halo, (alkyl)amino, cyano, CN, NCO], useful as adhesives, crosslinking agents or intermediates (no data), comprises hydrosilylation of alkenes R ₆ R ₅ C:CHR ₄ by silanes HSiR ₁ R ₂ R ₃ , preferably by chlorodimethylsilane, at 1:1.1 to 1:1.25 mol ratio, in the presence of iridium diene catalysts, preferably in the presence of di-μ-chlorobis[(1,2,5,6-η)-1,5- cyclooctadiene]diiridium and oxidative cocatalysts chosen from inorg. or organometallic oxidants, preferably ferrocenium, [Ru(bipy) ₃] ³⁺ and [Fe(phen) ₃] ³⁺ , organic oxidants chosen from aldehydes, ketones, diones peroxides, peracids, phosphine oxides, sulfones, tritylium and tropylium salts, taken in 0.5-5 wt% to the reactants, in a continuous reactor at 0-200°, preferably at 25-40° at 1-20 atm pressure, preferably as solvent-free process. In an example, a mixture of 0.562 mol of allyl chloride with 70 mg of [(cod)IrCl] ₂ was reacted with a mixture of 56 g of Me ₂ SiClH and 2 g of acetone as cocatalyst at 90° for 0.5 h, yielding 70% of chloro(3-chloropropyl)dimethylsilane.			
CC	29-6 (Organometallic and Organometalloidal Compounds) Section cross-reference(s): 45			
ST	silane alkyl prepn process hydrosilylation alkene iridium oxidant catalyst; alkylsilane improved process prepn alkene hydrosilylation oxidative cocatalyst; solvent free continuous process alkylsilane prepn iridium catalyzed hydrosilylation; ketone dione peroxide cocatalyst hydrosilylation iridium catalyst improved process			
IT	Silanes RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation) (alkoxy; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of alkenes catalyzed by iridium diene complexes and oxidative cocatalysts in continuous flow reactors and microreactors)			
IT	Silanes RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)			

(alkyl; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Ketones, uses

RL: CAT (Catalyst use); USES (Uses)

(diketones; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Reactors

(flow; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Hydrosilylation

Oxidizing agents

(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Aldehydes, uses

Ketones, uses

RL: CAT (Catalyst use); USES (Uses)

(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT **Alkenes**, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Reactors

(loop; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Reactors

(microreactors; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Peroxides, uses

RL: CAT (Catalyst use); USES (Uses)

(organic; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Carboxylic acids, uses

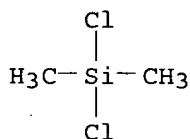
RL: CAT (Catalyst use); USES (Uses)

(peroxy; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Reactors

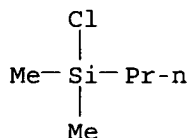
(tubular; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

- reactors and microreactors)
- IT 67-64-1, Acetone, uses 100-52-7, Benzaldehyde, uses 108-10-1, Methyl isobutyl ketone 110-05-4, Di-tert-butyl peroxide 123-54-6, Acetylacetone, uses 130-15-4, 1,4-Naphthoquinone 134-81-6, Benzil 504-02-9, 1,3-Cyclohexanedione 637-88-7, 1,4-Cyclohexanedione 765-87-7, 1,2-Cyclohexanedione 7553-56-2, Iodine, uses 7722-64-7, Potassium permanganate 7726-95-6, Bromine, uses 7775-27-1, Sodium peroxodisulfate 7778-50-9, Potassium bichromate 7782-44-7, Oxygen, uses 7782-50-5, Chlorine, uses 7789-00-6, Potassium chromate 10466-65-6, Potassium perrhenate 12125-80-3, Ferrocenium 13479-49-7 13746-66-2, Tripotassium hexacyanoferrate 18955-01-6 31067-25-1, 1,9-Cyclohexadecanedione
- RL: CAT (Catalyst use); USES (Uses)
(cocatalyst; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)
- IT 75-78-5P, Dichlorodimethylsilane 17477-29-1P, Chlorodimethylpropylsilane
- RL: BYP (Byproduct); PREP (Preparation)
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)
- IT 12112-67-3, Chloro(1,5-cyclooctadiene)iridium dimer
- RL: CAT (Catalyst use); USES (Uses)
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)
- IT 107-05-1, Allyl chloride 1066-35-9, Chlorodimethylsilane
- RL: RCT (Reactant); RACT (Reactant or reagent)
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)
- IT 10605-40-0P
- RL: SPN (Synthetic preparation); PREP (Preparation)
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)
- IT 75-78-5P, Dichlorodimethylsilane 17477-29-1P, Chlorodimethylpropylsilane
- RL: BYP (Byproduct); PREP (Preparation)
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)
- RN 75-78-5 HCAPLUS
- CN Silane, dichlorodimethyl- (8CI, 9CI) (CA INDEX NAME)



RN 17477-29-1 HCAPLUS

CN Silane, chlorodimethylpropyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



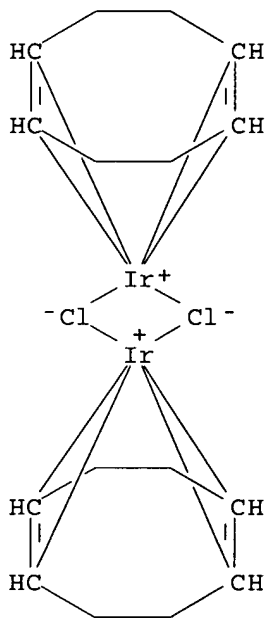
IT 12112-67-3, Chloro(1,5-cyclooctadiene)iridium dimer

RL: CAT (Catalyst use); USES (Uses)

(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

RN 12112-67-3 HCAPLUS

CN Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di- (9CI)
(CA INDEX NAME)



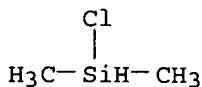
IT 1066-35-9, Chlorodimethylsilane

RL: RCT (Reactant); RACT (Reactant or reagent)

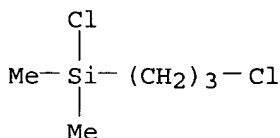
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

RN 1066-35-9 HCAPLUS

CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT 10605-40-0P
 RL: SPN (Synthetic preparation); **PREP (Preparation)**
 (improved process for preparation of alkylsilanes by solvent-free
 hydrosilylation of **alkenes** catalyzed by iridium **diene**
 complexes and oxidative cocatalysts in **continuous** flow
 reactors and microreactors)
 RN 10605-40-0 HCAPLUS
 CN Silane, chloro(3-chloropropyl)dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX
 NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 24 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2005:449533 HCAPLUS
 DOCUMENT NUMBER: 142:463198
 TITLE: Stabilization method of iridium catalyst solution
 INVENTOR(S): Tonomura, Yoichi; Kiyomori, Ayumu; Kubota, Toru
 PATENT ASSIGNEE(S): Shin-Etsu Chemical Industry Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005131454	A2	20050526	JP 2003-367190	20031028
PRIORITY APPLN. INFO.:			JP 2003-367190	20031028
OTHER SOURCE(S):	MARPAT 142:463198			

AB The invention refers to a stabilization method of an Ir catalyst solution
 used in hydrosilylation reactions, wherein a hydroxyl compound R1OH [R1 =
 C1-20 (un)substituted monovalent hydrocarbon] is added to the solution

IC ICM B01J033-00

ICS B01J031-22; C07F015-00

CC 21-2 (General Organic Chemistry)

Section cross-reference(s): 67

IT 64-17-5, Ethanol, uses 104-76-7, 2-Ethyl-1-hexanol 150-76-5,
 4-Methoxyphenol 12112-67-3

RL: **CAT (Catalyst use)**; DEV (Device component use); USES (Uses)
 (stabilization method of iridium catalyst solution)

IT 96-05-9, Allyl methacrylate 1066-35-9, Dimethylchlorosilane

RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
 (stabilization method of iridium catalyst solution)

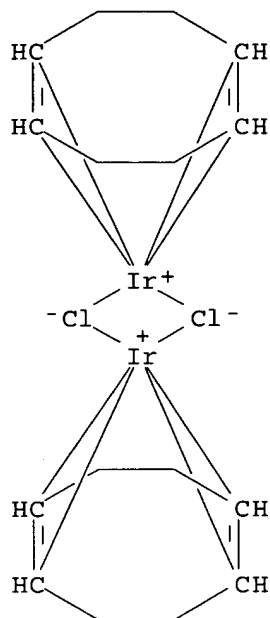
IT 24636-31-5P

RL: SPN (Synthetic preparation); **PREP (Preparation)**
 (stabilization method of iridium catalyst solution)

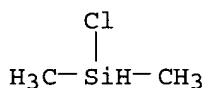
IT 12112-67-3

RL: **CAT (Catalyst use)**; DEV (Device component use); USES (Uses)
 (stabilization method of iridium catalyst solution)

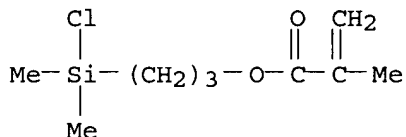
RN 12112-67-3 HCAPLUS
 CN Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di- (9CI)
 (CA INDEX NAME)



IT 1066-35-9, Dimethylchlorosilane
 RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
 (stabilization method of iridium catalyst solution)
 RN 1066-35-9 HCAPLUS
 CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT 24636-31-5P
 RL: SPN (Synthetic preparation); **PREP (Preparation)**
 (stabilization method of iridium catalyst solution)
 RN 24636-31-5 HCAPLUS
 CN 2-Propenoic acid, 2-methyl-, 3-(chlorodimethylsilyl)propyl ester (9CI)
 (CA INDEX NAME)



L64 ANSWER 25 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2005:1335585 HCAPLUS
 DOCUMENT NUMBER: 144:51711

TITLE: Improved process for controlled hydrolysis of residues from preparation of an ω -haloalkyl dialkylhalosilanes with subsequent regeneration of platinum-group metal catalyst

INVENTOR(S): Ramdani, Kamel

PATENT ASSIGNEE(S): Rhodia Chimie, Fr.

SOURCE: Fr. Demande, 19 pp.
CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2871802	A1	20051223	FR 2004-6502	20040616
WO 2006003323	A1	20060112	WO 2005-FR1469	20050614

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: FR 2004-6502 A 20040616

OTHER SOURCE(S): MARPAT 144:51711

AB ω -Haloalkyl dialkylhalosilanes of formula $\text{XR}_2\text{R}_3\text{Si}(\text{CH}_2)_s\text{X}$ [1, X = Cl, Br, I, preferably X = Cl; R₂, R₃ = C1-6 (un)branched alkyl, Ph; S = 2-10; preferably R₂ = R₃ = Me, s = 3] were prepared by hydrosilylation of **alkenes** $\text{CH}_2:\text{CH}(\text{CH}_2)_s-2\text{X}$ (same s, X) catalyzed by platinum-group metal compound, preferably of the type $[\text{Ir}(\text{R}_4)\text{X}]_2$ [R₄ = unsatd. C4-30 hydrocarbon having 1-8 double or triple bonds; same X]; the improved process, comprises separation of the reaction product 1 by distillation, controlled hydrolysis of the residue containing 40-50% of total halogen and 15-25% of ionizable halogen by addition of 1-5 mol (preferably 1-3 mol) of water per mol of hydrolyzable halogen (Y) at 40-60° with 0.002-0.015 mol H₂O min⁻¹ (mol Y)⁻¹, under stirring rate of 200-600 rpm and inert gas bubbling with the debit of 10-50 g h⁻¹. In an example, the controlled hydrolysis of the distillation residue containing 20% of hydrolyzable Cl (2.25 mol) and 1.2 wt%

of Ir catalyst at 50° was performed by addition of 120 g of H₂O (0.400 g min⁻¹ addition rate) in 1 L reactor with stirring at 400 rpm and bubbling of argon with 14 g h⁻¹ rate; the final content of Cl was 0.13 wt%. The invented method of hydrolysis produces monophasic product, from which the regeneration of Ir catalyst is may be performed without adsorption on solid adsorbent.

IC ICM C07F007-12

CC 29-6 (Organometallic and Organometalloidal Compounds)

IT 12111-11-4 12112-67-3, Di- μ -chlorobis(1,5-cyclooctadiene)diiridium 12245-73-7 60255-04-1 60255-25-6 60255-27-8 656240-93-6 656240-94-7 656240-95-8 656240-96-9

RL: CAT (Catalyst use); USES (Uses)

(improved process for controlled hydrolysis and hydrogen halide removal

in treatment of platinum-group metal catalyzed hydrosilylation residues)

IT 107-05-1, Allyl chloride 1066-35-9

RL: **RCT (Reactant); RACT (Reactant or reagent)**

(improved process for controlled hydrolysis and hydrogen halide removal in treatment of platinum-group metal catalyzed hydrosilylation residues)

IT 10605-40-0P

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(improved process for controlled hydrolysis and hydrogen halide removal in treatment of platinum-group metal catalyzed hydrosilylation residues)

IT 12111-11-4 12112-67-3, Di- μ -chlorobis(1,5-cyclooctadiene)diiridium 12245-73-7 60255-04-1

60255-25-6 60255-27-8 656240-93-6

656240-94-7 656240-95-8 656240-96-9

RL: **CAT (Catalyst use); USES (Uses)**

(improved process for controlled hydrolysis and hydrogen halide removal in treatment of platinum-group metal catalyzed hydrosilylation residues)

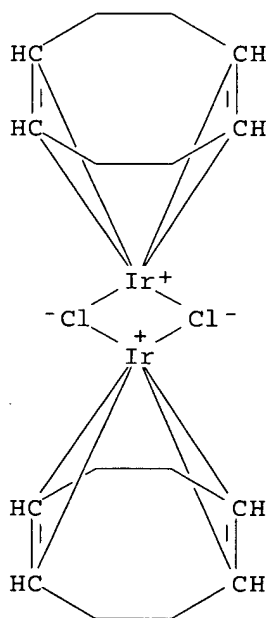
RN 12111-11-4 HCAPLUS

CN Iridium, bis[(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene]di- μ -chlorodi- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

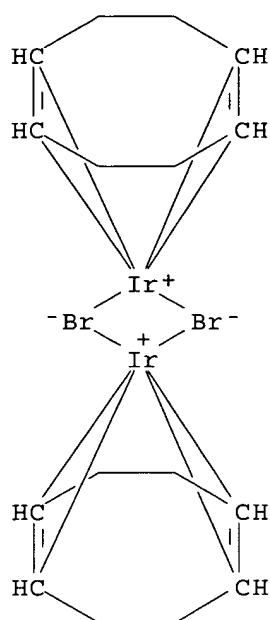
RN 12112-67-3 HCAPLUS

CN Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



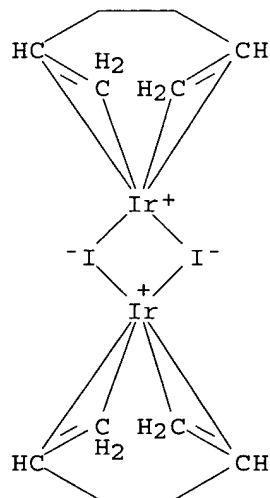
RN 12245-73-7 HCAPLUS

CN Iridium, di- μ -bromobis[(1,2,5,6- η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



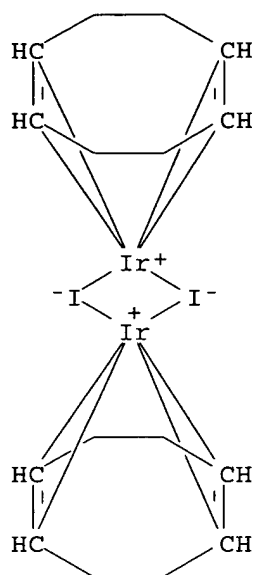
RN 60255-04-1 HCAPLUS

CN Iridium, bis[(1,2,5,6-η)-1,5-hexadiene]di-μ-iododi- (9CI) (CA
INDEX NAME)



RN 60255-25-6 HCAPLUS

CN Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-iododi- (9CI) (CA
INDEX NAME)



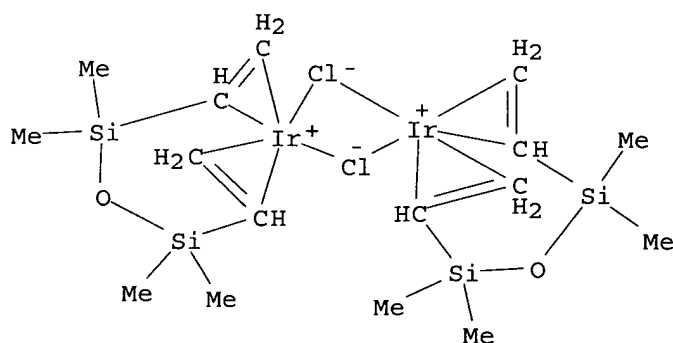
RN 60255-27-8 HCAPLUS

CN Iridium, bis[(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene]di- μ -iododi- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

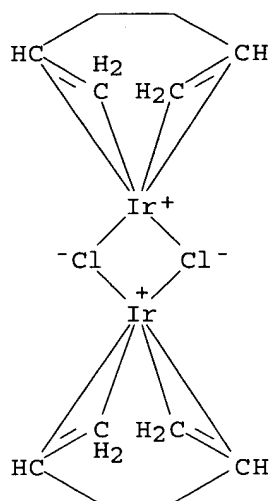
RN 656240-93-6 HCAPLUS

CN Iridium, di- μ -chlorobis(η^4 -1,3-diethenyl-1,1,3,3-tetramethyldisiloxane)di- (9CI) (CA INDEX NAME)

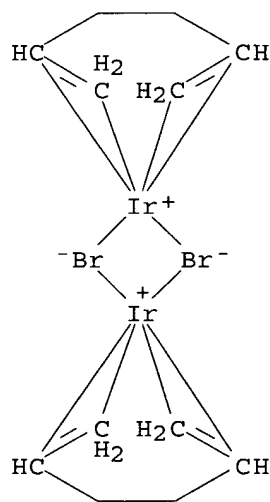


RN 656240-94-7 HCAPLUS

CN Iridium(2+), di- μ -chlorobis[(1,2,5,6- η)-1,5-hexadiene]di- (9CI) (CA INDEX NAME)



RN 656240-95-8 HCAPLUS
 CN Iridium, di- μ -bromobis[(1,2,5,6- η)-1,5-hexadiene]di- (9CI) (CA INDEX NAME)



RN 656240-96-9 HCAPLUS
 CN Iridium, bis[(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene]di- μ -bromodi- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

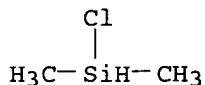
IT 1066-35-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(improved process for controlled hydrolysis and hydrogen halide removal in treatment of platinum-group metal catalyzed hydrosilylation residues)

RN 1066-35-9 HCAPLUS

CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

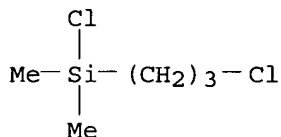


IT 10605-40-0P

RL: SPN (Synthetic preparation); **PREP (Preparation)**
(improved process for controlled hydrolysis and hydrogen halide removal
in treatment of platinum-group metal catalyzed hydrosilylation
residues)

RN 10605-40-0 HCAPLUS

CN Silane, chloro(3-chloropropyl)dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX
NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 26 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1089559 HCAPLUS

DOCUMENT NUMBER: 143:347293

TITLE: Preparation of (chloropropyl)trialkoxysilane from
trialkoxysilane

INVENTOR(S): Xu, Qimin; Xu, Chenggong; Zhang, Zhenglin; Yan,
Zeliang; Yang, Yaping

PATENT ASSIGNEE(S): Jurong Xingchun Chemical Co., Ltd., Peop. Rep. China;
Southeast University

SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 5 pp.
CODEN: CNXXEV

DOCUMENT TYPE: Patent

LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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CN 1563015	A	20050112	CN 2004-10014296	20040312
PRIORITY APPLN. INFO.:			CN 2004-10014296	20040312

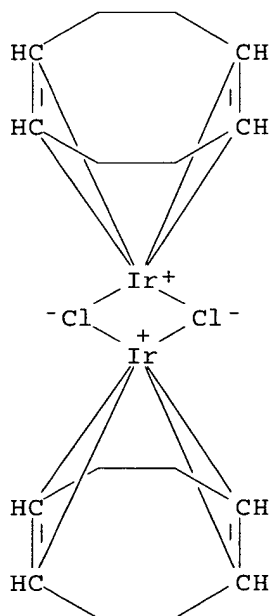
OTHER SOURCE(S): CASREACT 143:347293

AB The invention discloses a process for preparing chloropropyltrialkoxysilane directly from trialkoxysilane, which comprises adding weighted trialkoxysilane into silane solvent (0.2-2 times the mass of trialkoxysilane) in the presence of transition metal compound or its alc. solution as catalyst (1-1,000 ppm the mass of trialkoxysilane calculated on the basis of metal ion) and protective nitrogen, reacting for 1-10 h at room temperature, adding chloropropene 1/3-10/3 the mole number of trialkoxysilane, heating to 25-150°C to allow the reaction to proceed for 2-4 h, adding dropwise chloropropene 1/5-1/20 the mole number of trialkoxysilane, maintaining the temperature for 1-3 h, and separating to obtain the final product.

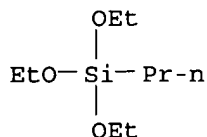
In the invention, the transition metal compound is used as catalyst to achieve homogeneous catalysis.

IC ICM C07F007-18

- CC 29-6 (Organometallic and Organometalloidal Compounds)
- IT 10025-83-9, Iridium chloride 10049-08-8, Ruthenium trichloride
12112-67-3, Cyclooctadiene iridium chloride dimer
 14996-61-3, Iridium trichloride hydrate 15243-33-1, Triruthenium
 dodecacarbonyl 16941-92-7, Chloroiridic acid 20765-98-4, Rhodium
 chloride hydrate
 RL: **CAT (Catalyst use)**; USES (Uses)
 (preparation of chloropropyltralkoxysilane by hydrosilylation of allyl
 chloride with trialkoxysilane in presence of transition metal compound)
- IT **29656-55-1P**, Chloropropyltriethoxysilane
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP**
(Preparation)
 (preparation of chloropropyltralkoxysilane by hydrosilylation of allyl
 chloride with trialkoxysilane in presence of transition metal compound)
- IT 107-05-1, Allyl chloride **998-30-1**, Triethoxysilane
 RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
 (preparation of chloropropyltralkoxysilane by hydrosilylation of allyl
 chloride with trialkoxysilane in presence of transition metal compound)
- IT **12112-67-3, Cyclooctadiene** iridium chloride dimer
 RL: **CAT (Catalyst use)**; USES (Uses)
 (preparation of chloropropyltralkoxysilane by hydrosilylation of allyl
 chloride with trialkoxysilane in presence of transition metal compound)
- RN 12112-67-3 HCAPLUS
- CN Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di- (9CI)
 (CA INDEX NAME)

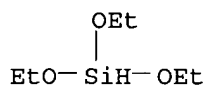


- IT **29656-55-1P**, Chloropropyltriethoxysilane
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP**
(Preparation)
 (preparation of chloropropyltralkoxysilane by hydrosilylation of allyl
 chloride with trialkoxysilane in presence of transition metal compound)
- RN 29656-55-1 HCAPLUS
- CN Silane, (chloropropyl)triethoxy- (9CI) (CA INDEX NAME)



D1-Cl

IT 998-30-1, Triethoxysilane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of chloropropyltralkoxysilane by hydrosilylation of allyl chloride with trialkoxysilane in presence of transition metal compound).
 RN 998-30-1 HCAPLUS
 CN Silane, triethoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)



L64 ANSWER 27 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2005:104757 HCAPLUS
 DOCUMENT NUMBER: 143:26955
 TITLE: Synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization
 AUTHOR(S): Pawluc, Piotr; Marciniec, Bogdan; Kownacki, Ireneusz; Maciejewski, Hieronim
 CORPORATE SOURCE: Department of Organometallic Chemistry, Faculty of Chemistry, Adam Mickiewicz University, Poznan, 60-780, Pol.
 SOURCE: Applied Organometallic Chemistry (2005), 19(1), 49-54
 CODEN: AOCHEX; ISSN: 0268-2605
 PUBLISHER: John Wiley & Sons Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB New phenylene-silylene-ethylene polymers were successfully synthesized using platinum-divinylsiloxane or rhodium and iridium siloxane complex-catalyzed polyhydrosilylation of divinylsubstituted carbosilanes with dihydrocarbosilanes or intermol. hydrosilylation of new hydrovinylcarbosilane. Polycarbosilanes have been obtained with high mol. wts. They seem to be potential parent substances for future applications as preceramic and membrane materials.
 CC 35-5 (Chemistry of Synthetic High Polymers)
 IT 11057-89-9 158240-74-5 448963-53-9 463967-39-7 681485-46-1
 RL: CAT (Catalyst use); USES (Uses)
 (synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)
 IT 106-37-6 1066-35-9 1637-65-6 1826-67-1 13528-93-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)
 IT 1719-58-0P 20152-11-8P 851479-30-6P
 852699-35-5P 852699-36-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)

IT **851479-31-7P 851479-32-8P 851479-33-9P**
852699-37-7P 852699-38-8P

RL: SPN (Synthetic preparation); **PREP (Preparation)**

(synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)

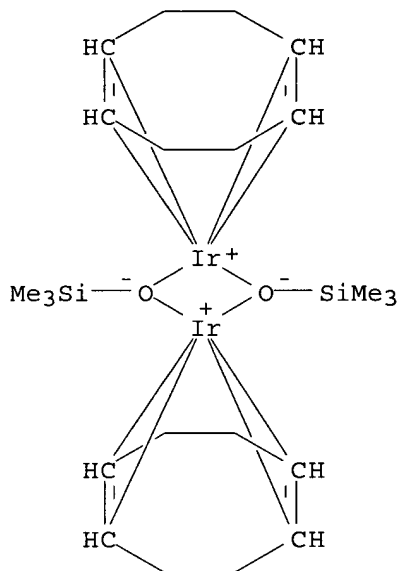
IT **448963-53-9**

RL: **CAT (Catalyst use)**; USES (Uses)

(synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)

RN 448963-53-9 HCAPLUS

CN Iridium, bis[(1,2,5,6- η)-1,5-cyclooctadiene]bis[μ -(trimethylsilanolato)]di- (9CI) (CA INDEX NAME)



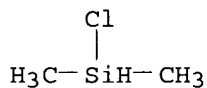
IT **1066-35-9**

RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**

(synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)

RN 1066-35-9 HCAPLUS

CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



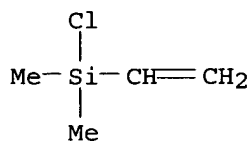
IT **1719-58-0P 20152-11-8P 851479-30-6P**
852699-35-5P 852699-36-6P

RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**

(synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)

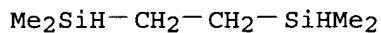
RN 1719-58-0 HCAPLUS

CN Silane, chloroethenyldimethyl- (9CI) (CA INDEX NAME)



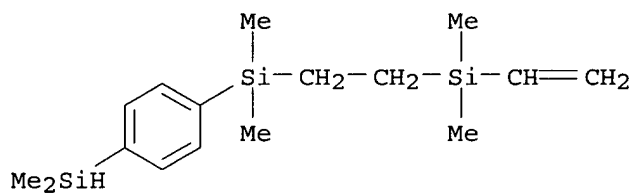
RN 20152-11-8 HCAPLUS

CN Silane, 1,2-ethanediylbis(dimethyl- (9CI) (CA INDEX NAME)



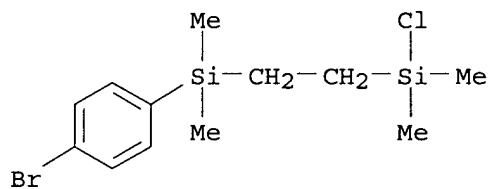
RN 851479-30-6 HCAPLUS

CN Silane, [4-(dimethylsilyl)phenyl][2-(ethenyldimethylsilyl)ethyl]dimethyl- (9CI) (CA INDEX NAME)



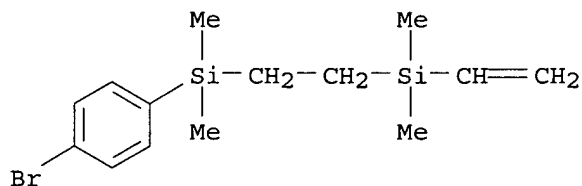
RN 852699-35-5 HCAPLUS

CN Silane, (4-bromophenyl)[2-(chlorodimethylsilyl)ethyl]dimethyl- (9CI) (CA INDEX NAME)



RN 852699-36-6 HCAPLUS

CN Silane, [2-[(4-bromophenyl)dimethylsilyl]ethyl]ethenyldimethyl- (9CI) (CA INDEX NAME)



IT 851479-31-7P 851479-32-8P 851479-33-9P

852699-37-7P 852699-38-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)

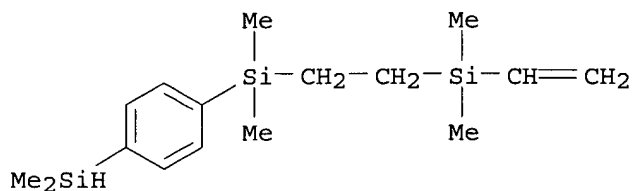
RN 851479-31-7 HCAPLUS

CN Silane, [4-(dimethylsilyl)phenyl][2-(ethenyldimethylsilyl)ethyl]dimethyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 851479-30-6

CMF C16 H30 Si3



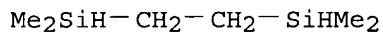
RN 851479-32-8 HCAPLUS

CN Silane, 1,2-ethanediylbis[dimethyl-, polymer with 1,4-phenylenebis[ethenyldimethylsilane] (9CI) (CA INDEX NAME)

CM 1

CRN 20152-11-8

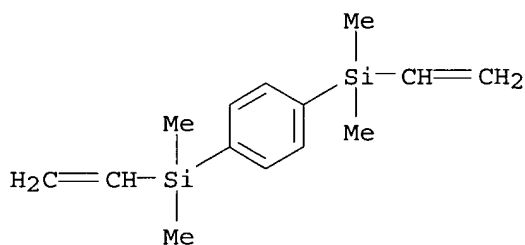
CMF C6 H18 Si2



CM 2

CRN 4519-17-9

CMF C14 H22 Si2



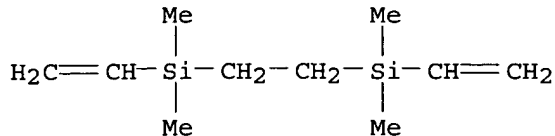
RN 851479-33-9 HCAPLUS

CN Silane, 1,2-ethanediylbis[ethenyldimethyl-, polymer with 1,4-phenylenebis[dimethylsilane] (9CI) (CA INDEX NAME)

CM 1

CRN 84677-98-5

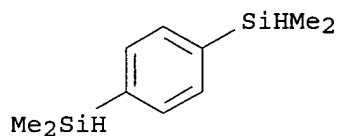
CMF C10 H22 Si2



CM 2

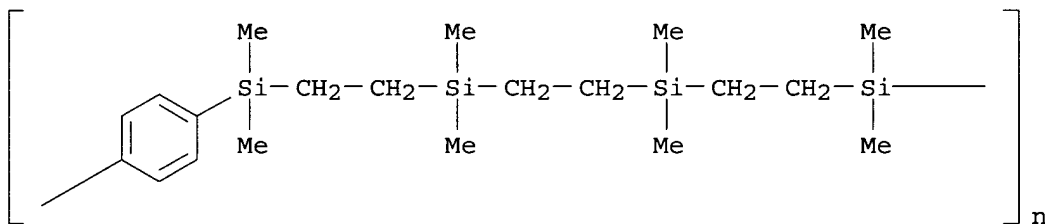
CRN 2488-01-9

CMF C10 H18 Si2



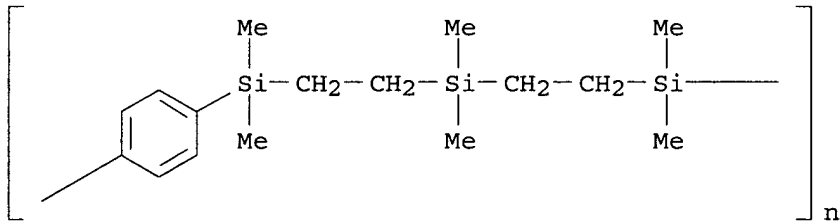
RN 852699-37-7 HCAPLUS

CN Poly[(dimethylsilylene)-1,2-ethanediyl(dimethylsilylene)-1,2-ethanediyl(dimethylsilylene)-1,2-ethanediyl(dimethylsilylene)-1,4-phenylene] (9CI) (CA INDEX NAME)



RN 852699-38-8 HCAPLUS

CN Poly[(dimethylsilylene)-1,2-ethanediyl(dimethylsilylene)-1,2-ethanediyl(dimethylsilylene)-1,4-phenylene] (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 28 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:120515 HCAPLUS

DOCUMENT NUMBER: 140:164015

TITLE: Process for preparation of haloalkyl(dialkyl)chlorosilanes by hydrosilylation of alkenyl halides in presence of iridium catalyst and subsequent catalyst recovery

INVENTOR(S): Guennouni, Nathalie; Ramdani, Kamel

PATENT ASSIGNEE(S): Rhodia Chimie, Fr.

SOURCE: Fr. Demande, 19 pp.
CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2843391	A1	20040213	FR 2002-10146	20020809
FR 2843391	B1	20040910		
FR 2843392	A1	20040213	FR 2003-284	20030113
FR 2843392	B1	20040910		
WO 2004016628	A1	20040226	WO 2003-FR2301	20030721
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003269042	A1	20040303	AU 2003-269042	20030721
EP 1554291	A1	20050720	EP 2003-750829	20030721
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRIORITY APPLN. INFO.:			FR 2002-10146	A 20020809
			FR 2003-284	A 20030113
			WO 2003-FR2301	W 20030721

OTHER SOURCE(S): MARPAT 140:164015

AB Haloalkyl(dialkyl)chlorosilanes XSi(RR1)(CH2)sX [X = Cl, Br, iodo; R, R1 = (un)branched C1-6 alkyl, Ph; s = 2-10] are prepared by hydrosilylation of alkenyl halides CH2:CH(CH2)s-2X (same X, s) with silanes XSi(RR1)H (same X, R, R1) in the presence of a platinum-group metal catalyst, preferably an iridium complex [Ir(R2)X]2 (same X, R2 = unsatd. C4-30 hydrocarbyl containing at least 1 C:C double bond and or C.tplbond.C triple bond), such that the reaction medium is distilled to sep. the product from distillation bottoms

comprising byproducts and the platinum-group metal or its derivs., whereupon the bottoms are contacted with a solid substance effective in adsorbing the platinum-group metal, and subsequent separation of the adsorbent from the platinum-group metal to recover the metal. Examples are given for recovery of catalysts based on Ir by using carbon black 2S as adsorbent following synthesis of 3-chloropropyl(dimethyl)chlorosilane.

IC ICM C07F007-14

CC 29-6 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 45

IT 7439-88-5P, Iridium, preparation 7440-04-2P, Osmium, preparation
7440-05-3P, Palladium, preparation 7440-06-4P, Platinum, preparation
7440-18-8P, Ruthenium, preparation 12111-11-4P
12112-67-3P 12245-73-7P 60255-04-1P
60255-25-6P 60255-27-8P 656240-93-6P

656240-94-7P 656240-95-8P 656240-96-9P

RL: CAT (Catalyst use); PUR (Purification or recovery); PREP (Preparation); USES (Uses)

(process for preparation of haloalkyl(dialkyl)chlorosilanes by hydrosilylation of alkenyl halides in presence of platinum-group catalyst and subsequent catalyst recovery)

IT 10605-40-0P, Chloro(3-chloropropyl)dimethylsilane

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(process for preparation of haloalkyl(dialkyl)chlorosilanes by hydrosilylation of alkenyl halides in presence of platinum-group catalyst and subsequent catalyst recovery)

IT 107-05-1, Allyl chloride 1066-35-9, Chloro(dimethyl)silane

RL: RCT (Reactant); RACT (Reactant or reagent)

(process for preparation of haloalkyl(dialkyl)chlorosilanes by hydrosilylation of alkenyl halides in presence of platinum-group catalyst and subsequent catalyst recovery)

IT 12111-11-4P 12112-67-3P 12245-73-7P

60255-04-1P 60255-25-6P 60255-27-8P

656240-93-6P 656240-94-7P 656240-95-8P

656240-96-9P

RL: CAT (Catalyst use); PUR (Purification or recovery); PREP (Preparation); USES (Uses)

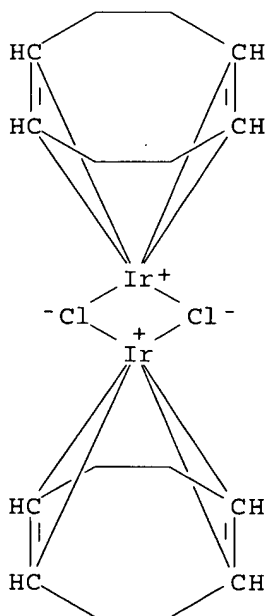
(process for preparation of haloalkyl(dialkyl)chlorosilanes by hydrosilylation of alkenyl halides in presence of platinum-group catalyst and subsequent catalyst recovery)

RN 12111-11-4 HCAPLUS

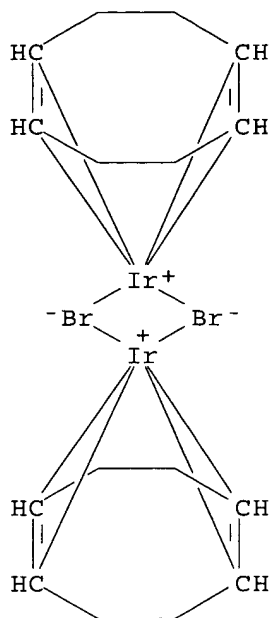
CN Iridium, bis[(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene]di- μ -chlorodi- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

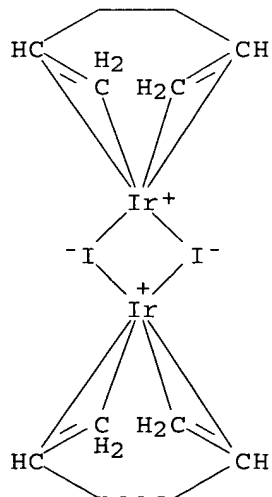
RN 12112-67-3 HCAPLUS

CN Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)

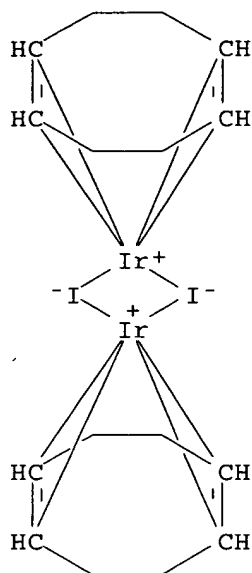
RN 12245-73-7 HCAPLUS
 CN Iridium, di- μ -bromobis[(1,2,5,6- η)-1,5-cyclooctadiene]di- (9CI)
 (CA INDEX NAME)



RN 60255-04-1 HCAPLUS
 CN Iridium, bis[(1,2,5,6- η)-1,5-hexadiene]di- μ -iododi- (9CI) (CA
 INDEX NAME)



RN 60255-25-6 HCAPLUS
 CN Iridium, bis[(1,2,5,6- η)-1,5-cyclooctadiene]di- μ -iododi- (9CI) (CA
 INDEX NAME)



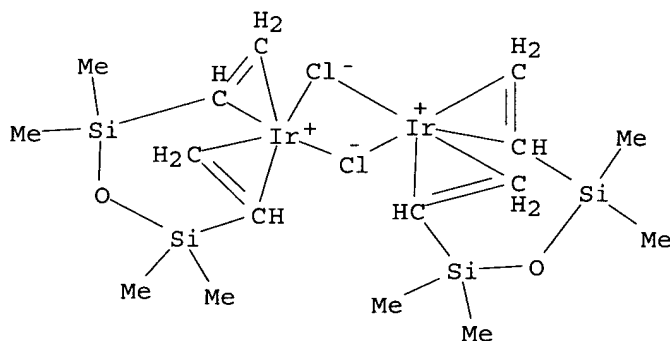
RN 60255-27-8 HCAPLUS

CN Iridium, bis[(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene]di-μ-iododi- (9CI) (CA INDEX NAME)

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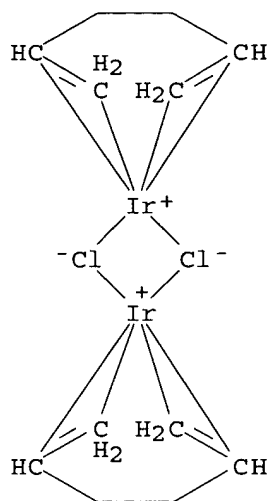
RN 656240-93-6 HCAPLUS

CN Iridium, di-μ-chlorobis(η⁴-1,3-diethenyl-1,1,3,3-tetramethyldisiloxane)di- (9CI) (CA INDEX NAME)



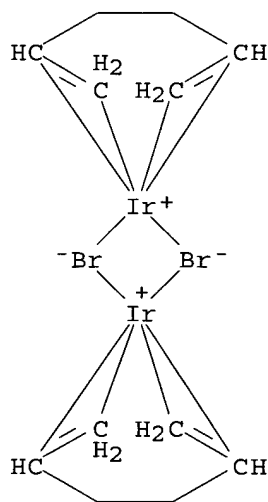
RN 656240-94-7 HCAPLUS

CN Iridium(2+), di-μ-chlorobis[(1,2,5,6-η)-1,5-hexadiene]di- (9CI) (CA INDEX NAME)



RN 656240-95-8 HCAPLUS

CN Iridium, di-μ-bromobis[(1,2,5,6-η)-1,5-hexadiene]di- (9CI) (CA INDEX NAME)



RN 656240-96-9 HCAPLUS

CN Iridium, bis[(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene]di-μ-bromodi- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

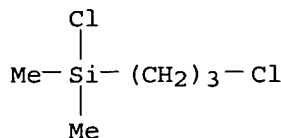
IT 10605-40-0P, Chloro(3-chloropropyl)dimethylsilane

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP** (Preparation)

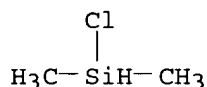
(process for preparation of haloalkyl(dialkyl)chlorosilanes by hydrosilylation of alkenyl halides in presence of platinum-group catalyst and subsequent catalyst recovery)

RN 10605-40-0 HCAPLUS

CN Silane, chloro(3-chloropropyl)dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 1066-35-9, Chloro(dimethyl)silane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (process for preparation of haloalkyl(dialkyl)chlorosilanes by
 hydrosilylation of alkenyl halides in presence of platinum-group
 catalyst and subsequent catalyst recovery)
 RN 1066-35-9 HCAPLUS
 CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 29 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2004:769875 HCAPLUS
 DOCUMENT NUMBER: 141:424227
 TITLE: Ru₃(CO)₁₂-Catalyzed Silylation of Benzylic C-H Bonds
 in Arylpyridines and Arylpyrazoles with Hydrosilanes
 via C-H Bond Cleavage
 AUTHOR(S): Kakiuchi, Fumitoshi; Tsuchiya, Kazuyuki; Matsumoto,
 Mitsutaka; Mizushima, Eiichiro; Chatani, Naoto
 CORPORATE SOURCE: Department of Applied Chemistry, Faculty of
 Engineering, Osaka University, Osaka, 565-0871, Japan
 SOURCE: Journal of the American Chemical Society (2004),
 126(40), 12792-12793
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:424227

AB Ruthenium-catalyzed silylation of sp³ C-H bonds at a benzylic position
 with hydrosilanes gave benzylsilanes. For this silylation reaction,
 Ru₃(CO)₁₂ complex showed high catalytic activity. This silylation
 proceeded at the Me C-H bond selectively. For this silylation reaction,
 pyridyl and pyrazolyl groups, and the imino group in hydrazones, can
 function as a directing group. Several hydrosilanes involving triethyl-,
 dimethylphenyl-, tert-butyldimethyl-, and triphenylsilanes can be used as
 a silylating reagent. Coordination of an sp² nitrogen atom to the
 ruthenium complex is important for achieving this silylation reaction.
 Thus, Ru₃(CO)₁₂/norbornene catalyzed silylation of 2-(2,6-
 dimethylphenyl)pyridine with Et₃SiH in PhMe at reflux gave 30%
 2-(2-methyl-6-triethylsilanylmethylphenyl)pyridine along with 55%
 2-(2,6-bis-triethylsilanylmethylphenyl)pyridine.
 CC 29-6 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 21
 IT 498-66-8, Norbornene 12148-71-9 13815-94-6, Ruthenium
 trichloride trihydrate 15243-33-1, Dodecacarbonyltriruthenium

19584-30-6, Tetrarhodium dodecacarbonyl 25360-32-1 52462-29-0
73468-85-6 91739-95-6 91947-90-9

RL: **CAT (Catalyst use)**; **USES (Uses)**

(ruthenium carbonyl catalyzed silylation of benzylic carbon-hydrogen bonds in arylpyridines and arylpyrazoles with hydrosilanes via carbon-hydrogen bond cleavage)

IT 611-32-5 **617-86-7**, Triethylsilane 766-77-8,
Dimethyl(phenyl)silane 789-25-3, Triphenylsilane 1762-32-9
10273-89-9 10273-91-3 10273-93-5 **29681-57-0**,
tert-Butyldimethylsilane 38581-14-5 706788-75-2 793681-25-1
793681-26-2 793681-27-3 793681-28-4 793681-29-5

RL: **RCT (Reactant)**; **RAC (Reactant or reagent)**

(ruthenium carbonyl catalyzed silylation of benzylic carbon-hydrogen bonds in arylpyridines and arylpyrazoles with hydrosilanes via carbon-hydrogen bond cleavage)

IT **793681-20-6P** **793681-21-7P** **793681-22-8P**
793681-23-9P **793681-24-0P** **793681-30-8P**
793681-31-9P **793681-32-0P** 793681-33-1P
793681-34-2P **793681-35-3P** **793681-36-4P**
793681-37-5P **793681-38-6P** **793681-39-7P**
793681-40-0P **793681-41-1P** **793681-42-2P**
793681-43-3P **793681-44-4P** **793681-45-5P**
793681-46-6P **793681-47-7P**

RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**

(ruthenium carbonyl catalyzed silylation of benzylic carbon-hydrogen bonds in arylpyridines and arylpyrazoles with hydrosilanes via carbon-hydrogen bond cleavage)

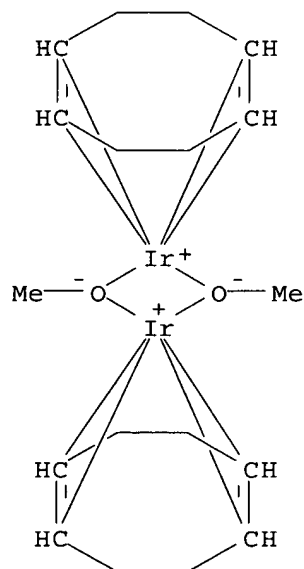
IT **12148-71-9**

RL: **CAT (Catalyst use)**; **USES (Uses)**

(ruthenium carbonyl catalyzed silylation of benzylic carbon-hydrogen bonds in arylpyridines and arylpyrazoles with hydrosilanes via carbon-hydrogen bond cleavage)

RN 12148-71-9 HCAPLUS

CN Iridium, bis[(1,2,5,6- η)-1,5-cyclooctadiene]di- μ -methoxydi- (9CI)
(CA INDEX NAME)



IT **617-86-7**, Triethylsilane **29681-57-0**,

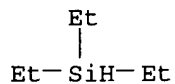
tert-Butyldimethylsilane

RL: RCT (Reactant); RACT (Reactant or reagent)

(ruthenium carbonyl catalyzed silylation of benzylic carbon-hydrogen bonds in arylpyridines and arylpyrazoles with hydrosilanes via carbon-hydrogen bond cleavage)

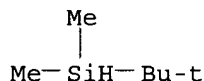
RN 617-86-7 HCAPLUS

CN Silane, triethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 29681-57-0 HCAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



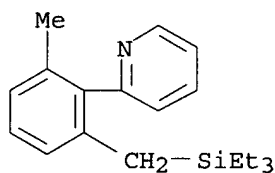
IT 793681-20-6P 793681-21-7P 793681-22-8P
 793681-23-9P 793681-24-0P 793681-30-8P
 793681-31-9P 793681-32-0P 793681-34-2P
 793681-35-3P 793681-36-4P 793681-37-5P
 793681-38-6P 793681-39-7P 793681-40-0P
 793681-41-1P 793681-42-2P 793681-43-3P
 793681-44-4P 793681-45-5P 793681-46-6P
 793681-47-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(ruthenium carbonyl catalyzed silylation of benzylic carbon-hydrogen bonds in arylpyridines and arylpyrazoles with hydrosilanes via carbon-hydrogen bond cleavage)

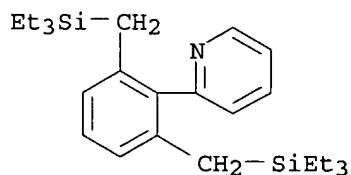
RN 793681-20-6 HCAPLUS

CN Pyridine, 2-[2-methyl-6-[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



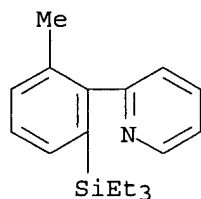
RN 793681-21-7 HCAPLUS

CN Pyridine, 2-[2,6-bis[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



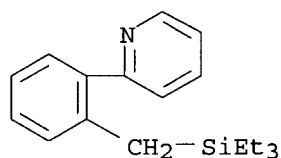
RN 793681-22-8 HCAPLUS

CN Pyridine, 2-[2-methyl-6-(triethylsilyl)phenyl]- (9CI) (CA INDEX NAME)



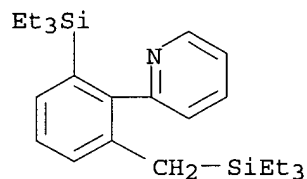
RN 793681-23-9 HCAPLUS

CN Pyridine, 2-[2-[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



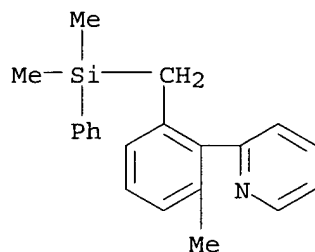
RN 793681-24-0 HCAPLUS

CN Pyridine, 2-[2-(triethylsilyl)-6-[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



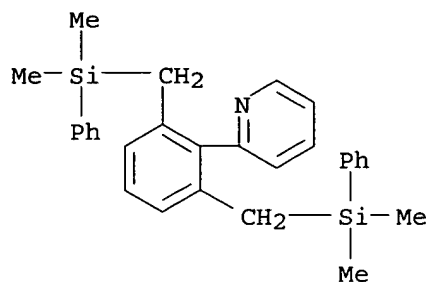
RN 793681-30-8 HCAPLUS

CN Pyridine, 2-[2-[(dimethylphenylsilyl)methyl]-6-methylphenyl]- (9CI) (CA INDEX NAME)



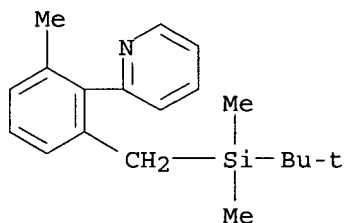
RN 793681-31-9 HCAPLUS

CN Pyridine, 2-[2,6-bis[(dimethylphenylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



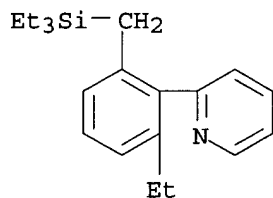
RN 793681-32-0 HCAPLUS

CN Pyridine, 2-[2-[[[1,1-dimethylethyl]dimethylsilyl]methyl]-6-methylphenyl]-(9CI) (CA INDEX NAME)



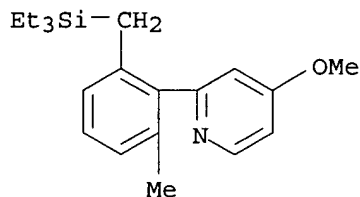
RN 793681-34-2 HCAPLUS

CN Pyridine, 2-[2-ethyl-6-[(triethylsilyl)methyl]phenyl]-(9CI) (CA INDEX NAME)



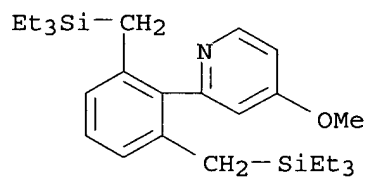
RN 793681-35-3 HCAPLUS

CN Pyridine, 4-methoxy-2-[2-methyl-6-[(triethylsilyl)methyl]phenyl]-(9CI) (CA INDEX NAME)



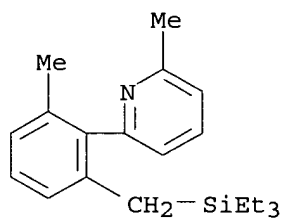
RN 793681-36-4 HCAPLUS

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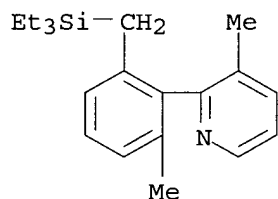
RN 793681-37-5 HCAPLUS

CN Pyridine, 2-methyl-6-[2-methyl-6-[(triethylsilyl)methyl]phenyl]- (9CI)
(CA INDEX NAME)



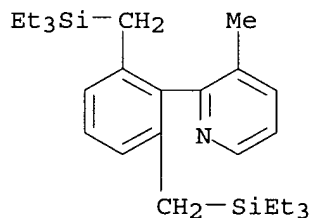
RN 793681-38-6 HCAPLUS

CN Pyridine, 3-methyl-2-[2-methyl-6-[(triethylsilyl)methyl]phenyl]- (9CI)
(CA INDEX NAME)



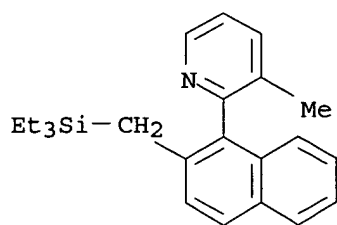
RN 793681-39-7 HCAPLUS

CN Pyridine, 2-[2,6-bis[(triethylsilyl)methyl]phenyl]-3-methyl- (9CI) (CA
INDEX NAME)



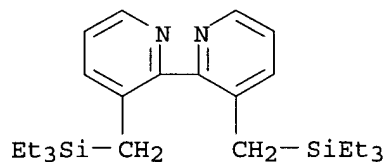
RN 793681-40-0 HCAPLUS

CN Pyridine, 3-methyl-2-[2-[(triethylsilyl)methyl]-1-naphthalenyl]- (9CI)
(CA INDEX NAME)



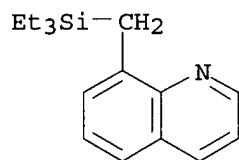
RN 793681-41-1 HCAPLUS

CN 2,2'-Bipyridine, 3,3'-bis[(triethylsilyl)methyl]- (9CI) (CA INDEX NAME)



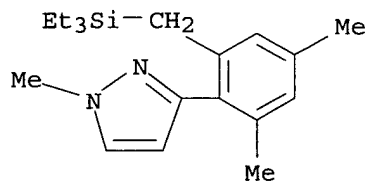
RN 793681-42-2 HCAPLUS

CN Quinoline, 8-[(triethylsilyl)methyl]- (9CI) (CA INDEX NAME)



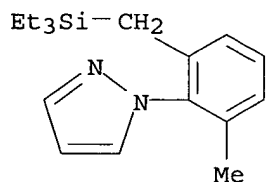
RN 793681-43-3 HCAPLUS

CN 1H-Pyrazole, 3-[2,4-dimethyl-6-[(triethylsilyl)methyl]phenyl]-1-methyl- (9CI) (CA INDEX NAME)

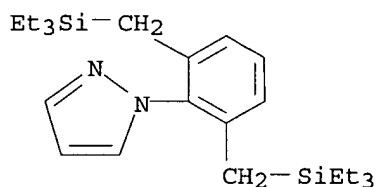


RN 793681-44-4 HCAPLUS

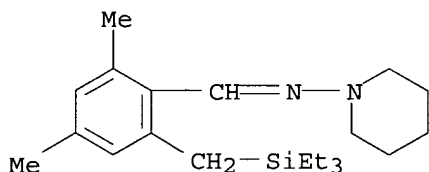
CN 1H-Pyrazole, 1-[2-methyl-6-[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



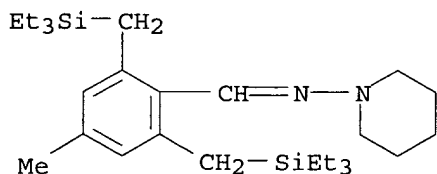
RN 793681-45-5 HCAPLUS
 CN 1H-Pyrazole, 1-[2,6-bis[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



RN 793681-46-6 HCAPLUS
 CN 1-Piperidinamine, N-[[2,4-dimethyl-6-[(triethylsilyl)methyl]phenyl]methyle
 ne]- (9CI) (CA INDEX NAME)



RN 793681-47-7 HCAPLUS
 CN 1-Piperidinamine, N-[[4-methyl-2,6-bis[(triethylsilyl)methyl]phenyl]methyle
 ne]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 30 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:16299 HCAPLUS

DOCUMENT NUMBER: 138:136796

TITLE: Selective, Catalytic Carbon-Carbon Bond Activation and
 Functionalization Promoted by Late Transition Metal
 Catalysts

AUTHOR(S): Bart, Suzanne C.; Chirik, Paul J.

CORPORATE SOURCE: Department of Chemistry and Chemical Biology Baker
Laboratory, Cornell University, Ithaca, NY, 14853, USA

SOURCE: Journal of the American Chemical Society (2003),
125(4), 886-887
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:136796

AB The selective catalytic activation and functionalization of carbon-carbon bonds in a series of substituted cyclopropane substrates has been developed using com. available transition metal catalysts. Catalytic hydrogenation and olefination procedures, tolerant of a range of functional groups, have been discovered. Introduction of a chelate-assisting substituent such as [PPh₂] is effective in altering the kinetic selectivity and lowering the activation barrier for the catalytic processes.

CC 22-4 (Physical Organic Chemistry)
Section cross-reference(s): 67

IT 12080-32-9, Dichloro(1,5-**cyclooctadiene**)platinum 12092-47-6,
Dichlorobis(1,5-**cyclooctadiene**)rhodium(I) 12112-67-3,
Dichlorobis(**cyclooctadiene**)diiridium 12246-51-4,
Dichlorotetrakis(cyclooctene)diiridium 13938-94-8,
Chlorocarbonylbis(triphenylphosphine)rhodium 14221-01-3,
Tetrakis(triphenylphosphine)palladium 14694-95-2, Rhodium
tris(triphenylphosphine) chloride
RL: **CAT (Catalyst use)**; **USES (Uses)**
(selective catalytic carbon-carbon bond activation and
functionalization promoted by transition metal catalysts)

IT 64-67-5, Diethylsulfate 75-36-5, Acetyl chloride 75-77-4,
Trimethylsilyl chloride, reactions 617-86-7, Triethylsilane
930-57-4 1079-66-9, Chlorodiphenylphosphine 2516-33-8,
Cyclopropanemethanol 25267-27-0, Iodobutane 473734-58-6
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(selective catalytic carbon-carbon bond activation and
functionalization promoted by transition metal catalysts)

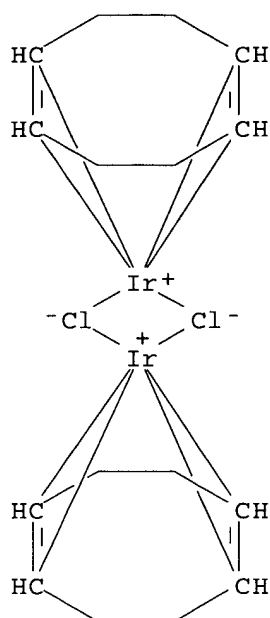
IT 36982-54-4P 70097-81-3P **85696-54-4P** 494769-09-4P
494769-10-7P
RL: **RCT (Reactant)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**; **RACT (Reactant or reagent)**
(selective catalytic carbon-carbon bond activation and
functionalization promoted by transition metal catalysts)

IT 78-83-1P, preparation 110-19-0P 591-76-4P 627-02-1P 820-71-3P
6094-02-6P 17616-98-7P **18269-50-6P** 24309-28-2P
25195-85-1P 494769-11-8P **494769-12-9P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(selective catalytic carbon-carbon bond activation and
functionalization promoted by transition metal catalysts)

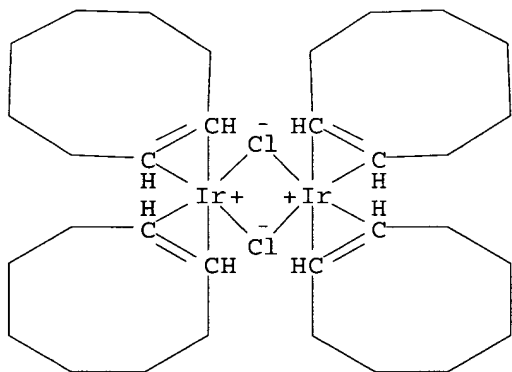
IT 12112-67-3, Dichlorobis(**cyclooctadiene**)diiridium
12246-51-4, Dichlorotetrakis(cyclooctene)diiridium
RL: **CAT (Catalyst use)**; **USES (Uses)**
(selective catalytic carbon-carbon bond activation and
functionalization promoted by transition metal catalysts)

RN 12112-67-3 HCAPLUS

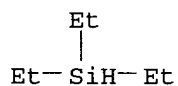
CN Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di- (9CI)
(CA INDEX NAME)



RN 12246-51-4 HCAPLUS
 CN Iridium, di- μ -chlorotetrakis[(1,2- η)-cyclooctene]di- (9CI) (CA INDEX NAME)



IT 617-86-7, Triethylsilane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (selective catalytic carbon-carbon bond activation and
 functionalization promoted by transition metal catalysts)
 RN 617-86-7 HCAPLUS
 CN Silane, triethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

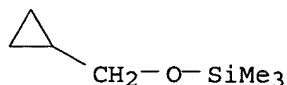


IT 85696-54-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)
 (selective catalytic carbon-carbon bond activation and
 functionalization promoted by transition metal catalysts)

RN 85696-54-4 HCAPLUS

CN Silane, (cyclopropylmethoxy)trimethyl- (9CI) (CA INDEX NAME)

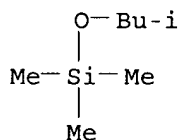


IT 18269-50-6P 25195-85-1P 494769-12-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (selective catalytic carbon-carbon bond activation and
 functionalization promoted by transition metal catalysts)

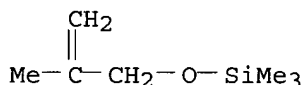
RN 18269-50-6 HCAPLUS

CN Silane, trimethyl(2-methylpropoxy)- (9CI) (CA INDEX NAME)



RN 25195-85-1 HCAPLUS

CN Silane, trimethyl[(2-methyl-2-propenyl)oxy]- (9CI) (CA INDEX NAME)



RN 494769-12-9 HCAPLUS

CN Phosphinous acid, diphenyl-, 4-(triethylsilyl)butyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 31 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:71112 HCAPLUS

DOCUMENT NUMBER: 137:47249

TITLE: The effect of oxygen on the regioselectivity in the
 rhodium catalysed hydrosilylation of 1,3-
dienes

AUTHOR(S): Gustafsson, Magnus; Frejd, Torbjorn

CORPORATE SOURCE: Organic Chemistry, Centre for Chemistry and Chemical
 Engineering, Lund University, Lund, S-221 00, Swed.

SOURCE: Journal of the Chemical Society, Perkin Transactions 1
 (2002), (1), 102-107

CODEN: JCSPCE; ISSN: 1472-7781

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 137:47249

- AB The regioselectivity of the hydrosilylation of substituted 1,3-**dienes** catalyzed by several Rh complexes in the presence and absence of O₂ was studied. In addition to the already known accelerating effect, the presence of O₂ strongly affected the product distribution. For 2-substituted 1,3-**dienes** in the presence of O₂ the regioselectivity was in the range of 1:6 to 1:10 in favor of the head-product, while the absence of O₂ changed the ratios to 1:1 to 3:1 in favor of the tail-product. When HSiPh₃ was used in the presence of O₂ a single isomer was isolated in 87% yield, while in the absence of O₂ a mixture of products was produced. Control expts. indicated that a heterogeneous/colloidal catalytic system may be responsible for the preferred head-product formation.
- CC 29-6 (Organometallic and Organometalloidal Compounds)
- ST oxygen effect regioselectivity rhodium catalyzed hydrosilylation unsym **diene**
- IT **Alkadienes**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (1,3-; effect of oxygen on regioselectivity in rhodium catalyzed hydrosilylation of unsym. **dienes**)
- IT Hydrosilylation
 Hydrosilylation catalysts
 Regiochemistry
 (effect of oxygen on regioselectivity in rhodium catalyzed hydrosilylation of unsym. **dienes**)
- IT **12112-67-3**, Dichlorobis(1,5-**cyclooctadiene**)diiridium
 RL: CAT (Catalyst use); USES (Uses)
 (effect of oxygen on regioselectivity in catalyzed hydrosilylation of unsym. **diene**)
- IT 13569-65-8, Rhodium trichloride trihydrate 13938-94-8, Carbonyl(chloro)bis(triphenylphosphine)rhodium 14284-92-5, Rhodium tris(acetylacetonate) 14694-95-2, Chlorotris(triphenylphosphine)rhodium 17185-29-4, Carbonylhydrotris(triphenylphosphine)rhodium 18284-36-1, Hydrotetrakis(triphenylphosphine)rhodium 26500-10-7, Chloro(thiocarbonyl)bis(triphenylphosphine)rhodium
 RL: CAT (Catalyst use); USES (Uses)
 (effect of oxygen on regioselectivity in rhodium catalyzed hydrosilylation of unsym. **diene**)
- IT 78-79-5, Isoprene, reactions 123-35-3, 7-Methyl-3-(methylene)-1,6-**octadiene** **617-86-7**, Triethylsilane 766-77-8, Dimethyl(phenyl)silane 789-25-3, Triphenylsilane 926-54-5, (E)-2-Methyl-1,3-**pentadiene** 930-68-7, 2-Cyclohexen-1-one **998-30-1**, Triethoxysilane 2004-70-8, (E)-1,3-**Pentadiene** **2487-90-3**, Trimethoxysilane 29414-55-9, 2,2-Dimethyl-3-(3-(methylene)-4-pentenyl)oxirane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (effect of oxygen on regioselectivity in rhodium catalyzed hydrosilylation of unsym. **diene**)
- IT **18032-09-2P**, 1-Triethylsilyl-3-methylbut-2-ene **35754-76-8P**, 1-Triethoxysilyl-3-methylbut-2-ene **50598-99-7P**, **63942-83-6P**, (Z)-1-Triethoxysilyl-2-methylbut-2-ene **63972-14-5P**, 1-[Dimethyl(phenyl)silyl]-3-methylbut-2-ene **68260-36-6P**, (E)-3,7-Dimethyl-1-[dimethyl(phenyl)silyl]octa-2,6-**diene** **72142-16-6P**, 1-Trimethoxysilyl-3-methylbut-2-ene **108311-91-7P**, (Z)-1-Triethylsilyl-2-methylbut-2-ene **108311-92-8P**, (Z)-1-Trimethoxysilyl-2-methylbut-2-ene **167314-58-1P**, (Z)-1-[Dimethyl(phenyl)silyl]-2-methylpent-2-ene **438045-62-6P**, (2Z)-1-Cyclohexyl-7-methyl-3-

[dimethyl(phenyl)silylmethyl]octa-2,6-**diene** 438045-63-7P,
 3-Methyl-1-triphenylsilylbut-2-ene 438045-64-8P, (Z)-1-(Triphenylsilyl)-
 2-methylbut-2-ene 438045-65-9P, (Z)-3-
 [Dimethyl(phenyl)silylmethyl]-7-methylocta-2,6-**diene**
 438045-66-0P, (E)-2,3-Epoxy-8-[dimethyl(phenyl)silyl]-2,6-
 dimethyloct-6-ene 438045-67-1P, (Z)-2,3-Epoxy-6-
 [dimethyl(phenyl)silylmethyl]-2-methyloct-6-ene 438045-68-2P,
 Dimethyl((E)-2-pentenyl)(phenyl)silane 438045-69-3P,
 1-[Dimethyl(phenyl)silyl]pent-2-ene 438045-70-6P,
 (2-(2-Cyclohexylethylidene)-6-methyl-5-heptenyl)dimethyl(phenyl)silane
 RL: SPN (Synthetic preparation); **PREP (Preparation)**
 (effect of oxygen on regioselectivity in rhodium catalyzed
 hydrosilylation of unsym. **diene**)

IT 438045-60-4P, (1E)-1-Cyclohexyl-7-methyl-3-oxoocta-1,6-**diene**
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT
 (Reactant or reagent)
 (preparation and Wittig reaction of)

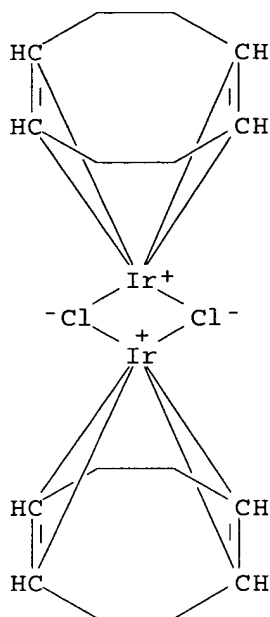
IT 438045-61-5P, (1E)-1-Cyclohexyl-7-methyl-3-methylenoocta-1,6-**diene**
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT
 (Reactant or reagent)
 (preparation and effect of oxygen on regioselectivity in rhodium catalyzed
 hydrosilylation of)

IT 12092-47-6, Bis(chloro(1,5-**cyclooctadiene**)rhodium)
 RL: CAT (Catalyst use); **USES (Uses)**
 (with phosphine; effect of oxygen on regioselectivity in rhodium
 catalyzed hydrosilylation of unsym. **diene**)

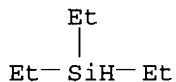
IT 603-35-0, Triphenylphosphine, uses
 RL: CAT (Catalyst use); **USES (Uses)**
 (with rhodium chloro **diene** complex; effect of oxygen on
 regioselectivity in rhodium catalyzed hydrosilylation of unsym.
diene)

IT 12112-67-3, Dichlorobis(1,5-**cyclooctadiene**)diiridium
 RL: **CAT (Catalyst use)**; **USES (Uses)**
 (effect of oxygen on regioselectivity in catalyzed hydrosilylation of
 unsym. **diene**)

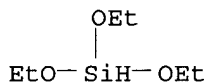
RN 12112-67-3 HCAPLUS
 CN Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di- (9CI)
 (CA INDEX NAME)



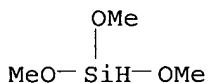
IT 617-86-7, Triethylsilane 998-30-1, Triethoxysilane
 2487-90-3, Trimethoxysilane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (effect of oxygen on regioselectivity in rhodium catalyzed
 hydrosilylation of unsym. diene)
 RN 617-86-7 HCAPLUS
 CN Silane, triethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 998-30-1 HCAPLUS
 CN Silane, triethoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)

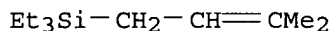


RN 2487-90-3 HCAPLUS
 CN Silane, trimethoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

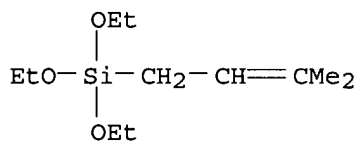


IT 18032-09-2P, 1-Triethylsilyl-3-methylbut-2-ene 35754-76-8P
 , 1-Triethoxysilyl-3-methylbut-2-ene 50598-99-7P
 63942-83-6P, (Z)-1-Triethoxysilyl-2-methylbut-2-ene

63972-14-5P, 1-[Dimethyl(phenyl)silyl]-3-methylbut-2-ene
 68260-36-6P, (E)-3,7-Dimethyl-1-[dimethyl(phenyl)silyl]octa-2,6-
diene 72142-16-6P, 1-Trimethoxysilyl-3-methylbut-2-ene
 108311-91-7P, (Z)-1-Triethylsilyl-2-methylbut-2-ene
 108311-92-8P, (Z)-1-Trimethoxysilyl-2-methylbut-2-ene
 167314-58-1P, (Z)-1-[Dimethyl(phenyl)silyl]-2-methylpent-2-ene
 438045-62-6P, (2Z)-1-Cyclohexyl-7-methyl-3-
 [dimethyl(phenyl)silylmethyl]octa-2,6-**diene** 438045-65-9P
 , (Z)-3-[Dimethyl(phenyl)silylmethyl]-7-methylocta-2,6-**diene**
 438045-66-0P, (E)-2,3-Epoxy-8-[dimethyl(phenyl)silyl]-2,6-
 dimethyloct-6-ene 438045-67-1P, (Z)-2,3-Epoxy-6-
 [dimethyl(phenyl)silylmethyl]-2-methyloct-6-ene 438045-68-2P,
 Dimethyl((E)-2-pentenyl)(phenyl)silane 438045-69-3P,
 1-[Dimethyl(phenyl)silyl]pent-2-ene 438045-70-6P,
 (2-(2-Cyclohexylethylidene)-6-methyl-5-heptenyl)dimethyl(phenyl)silane
 RL: SPN (Synthetic preparation); **PREP (Preparation)**
 (effect of oxygen on regioselectivity in rhodium catalyzed
 hydrosilylation of unsym. **diene**)
 RN 18032-09-2 HCAPLUS
 CN Silane, triethyl(3-methyl-2-butenyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)

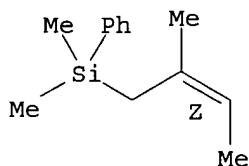


RN 35754-76-8 HCAPLUS
 CN Silane, triethoxy(3-methyl-2-butenyl)- (9CI) (CA INDEX NAME)



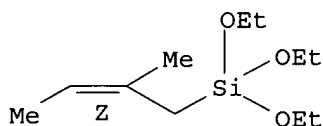
RN 50598-99-7 HCAPLUS
 CN Silane, dimethyl[(2Z)-2-methyl-2-butenyl]phenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



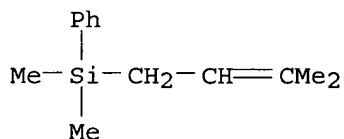
RN 63942-83-6 HCAPLUS
 CN Silane, triethoxy[(2Z)-2-methyl-2-butenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 63972-14-5 HCAPLUS

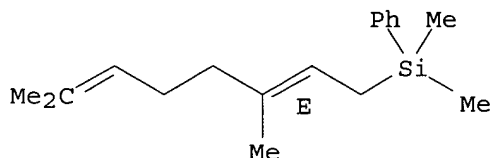
CN Silane, dimethyl(3-methyl-2-butenyl)phenyl- (9CI) (CA INDEX NAME)



RN 68260-36-6 HCAPLUS

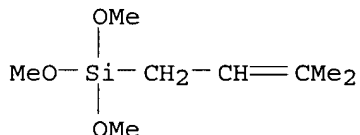
CN Silane, [(2E)-3,7-dimethyl-2,6-octadienyl]dimethylphenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 72142-16-6 HCAPLUS

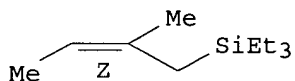
CN Silane, trimethoxy(3-methyl-2-butenyl)- (9CI) (CA INDEX NAME)



RN 108311-91-7 HCAPLUS

CN Silane, triethyl[(2Z)-2-methyl-2-butenyl]- (9CI) (CA INDEX NAME)

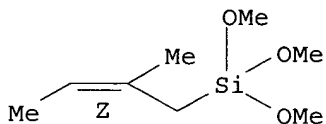
Double bond geometry as shown.



RN 108311-92-8 HCAPLUS

CN Silane, trimethoxy[(2Z)-2-methyl-2-butenyl]- (9CI) (CA INDEX NAME)

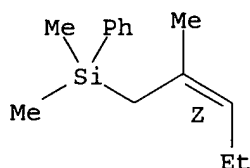
Double bond geometry as shown.



RN 167314-58-1 HCAPLUS

CN Silane, dimethyl[(2Z)-2-methyl-2-pentenyl]phenyl- (9CI) (CA INDEX NAME)

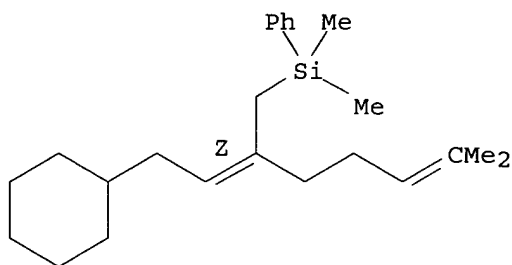
Double bond geometry as shown.



RN 438045-62-6 HCAPLUS

CN Silane, [(2Z)-2-(2-cyclohexylethylidene)-6-methyl-5-heptenyl]dimethylphenyl- (9CI) (CA INDEX NAME)

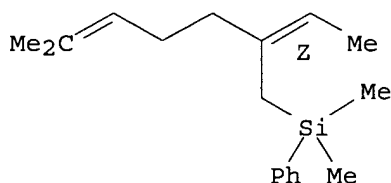
Double bond geometry as shown.



RN 438045-65-9 HCAPLUS

CN Silane, [(2Z)-2-ethylidene-6-methyl-5-heptenyl]dimethylphenyl- (9CI) (CA INDEX NAME)

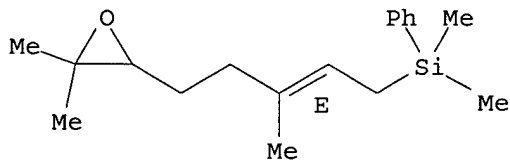
Double bond geometry as shown.



RN 438045-66-0 HCAPLUS

CN Silane, [(2E)-5-(3,3-dimethyloxiranyl)-3-methyl-2-pentenyl]dimethylphenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

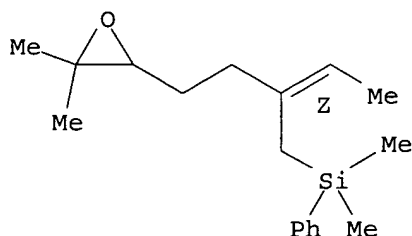


RN 438045-67-1 HCAPLUS

CN Silane, [(2Z)-2-[2-(3,3-dimethyloxiranyl)ethyl]-2-butenyl]dimethylphenyl-

(9CI) (CA INDEX NAME)

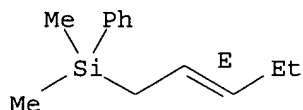
Double bond geometry as shown.



RN 438045-68-2 HCAPLUS

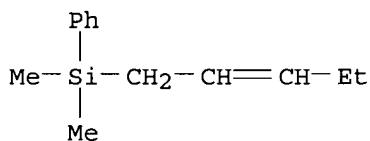
CN Silane, dimethyl-(2E)-2-pentenylphenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



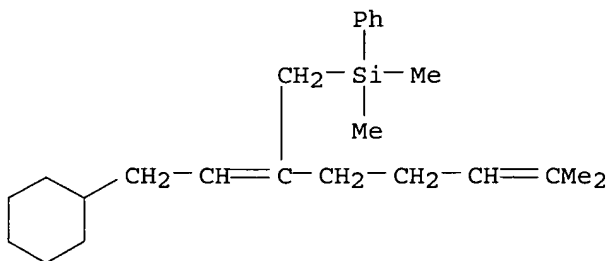
RN 438045-69-3 HCAPLUS

CN Silane, dimethyl-2-pentenylphenyl- (9CI) (CA INDEX NAME)



RN 438045-70-6 HCAPLUS

CN Silane, [2-(2-cyclohexylethylidene)-6-methyl-5-heptenyl]dimethylphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 32 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:128366 HCAPLUS

DOCUMENT NUMBER: 132:251176

TITLE: Dehydrogenative silylation of terminal alkynes by iridium catalyst

AUTHOR(S): Shimizu, Rie; Fuchikami, Takamasa
 CORPORATE SOURCE: Sagami Chemical Research Center, Kanagawa, 229-0012, Japan
 SOURCE: Tetrahedron Letters (2000), 41(6), 907-910
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Dehydrogenative silylation of terminal alkynes with hydrosilanes proceeds in the presence of Ir catalyst to afford the corresponding silylacetylenes. When phenylacetylene and triethylsilane were heated in dry DME in the presence of Ir₄(CO)₁₂PPh₃, (2-phenylethynyl)triethylsilane was obtained in 96% yield with little of hydrosilylated products. The present method is applicable for a variety of terminal alkynes and hydrosilanes to give the corresponding silylacetylenes in good yields with high selectivities.

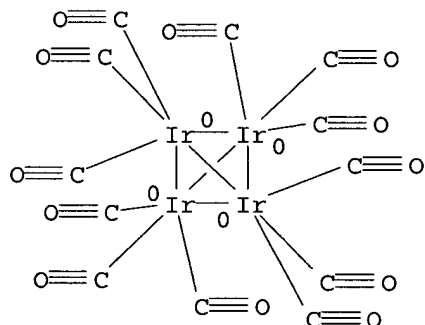
CC 29-6 (Organometallic and Organometalloidal Compounds)
 IT 603-35-0, Triphenylphosphine, uses 18827-81-1, Tetrairidium dodecacarbonyl
 RL: CAT (Catalyst use); USES (Uses)
 (dehydrogenative silylation of terminal alkynes by iridium catalyst)

IT 536-74-3, Phenylacetylene 617-86-7, Triethylsilane 629-05-0, 1-Octyne 766-77-8, Dimethylphenylsilane 917-92-0, 3,3-Dimethyl-1-butyne 931-48-6, Cyclohexylacetylene 1438-82-0, Dimethyl(trimethylsiloxy)silane 14857-34-2, Ethoxydimethylsilane 29681-57-0, tert-Butyldimethylsilane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (dehydrogenative silylation of terminal alkynes by iridium catalyst)

IT 1081-97-6P 4131-43-5P, Triethyl(phenylethynyl)silane 18408-64-5P, Triethyl-1-octynylsilane 75573-29-4P 79628-15-2P, Dimethylphenyl(phenylethynyl)silane 85443-40-9P, tert-Butyldimethyl(phenylethynyl)silane 146139-33-5P, Ethoxydimethyl(phenylethynyl)silane 148991-61-1P, Cyclohexylethynyltriethylsilane
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (dehydrogenative silylation of terminal alkynes by iridium catalyst)

IT 18827-81-1, Tetrairidium dodecacarbonyl
 RL: CAT (Catalyst use); USES (Uses)
 (dehydrogenative silylation of terminal alkynes by iridium catalyst)

RN 18827-81-1 HCAPLUS
 CN Iridium, dodecacarbonyltetra-, tetrahedro (9CI) (CA INDEX NAME)

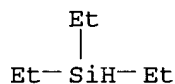


IT 617-86-7, Triethylsilane 14857-34-2, Ethoxydimethylsilane 29681-57-0, tert-Butyldimethylsilane
 RL: RCT (Reactant); RACT (Reactant or reagent)

(dehydrogenative silylation of terminal alkynes by iridium catalyst)

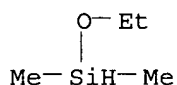
RN 617-86-7 HCAPLUS

CN Silane, triethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



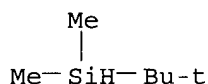
RN 14857-34-2 HCAPLUS

CN Silane, ethoxydimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 29681-57-0 HCAPLUS

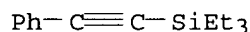
CN Silane, (1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



IT 4131-43-5P, Triethyl(phenylethynyl)silane 18408-64-5P,
 Triethyl-1-octynylsilane 75573-29-4P 79628-15-2P,
 Dimethylphenyl(phenylethynyl)silane 85443-40-9P,
 tert-Butyldimethyl(phenylethynyl)silane 146139-33-5P,
 Ethoxydimethyl(phenylethynyl)silane 148991-61-1P,
 Cyclohexylethynyltriethylsilane
 RL: SPN (Synthetic preparation); **PREP (Preparation)**
 (dehydrogenative silylation of terminal alkynes by iridium catalyst)

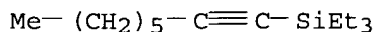
RN 4131-43-5 HCAPLUS

CN Silane, triethyl(phenylethynyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)



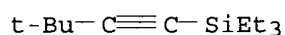
RN 18408-64-5 HCAPLUS

CN Silane, triethyl-1-octynyl- (8CI, 9CI) (CA INDEX NAME)



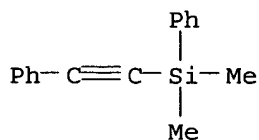
RN 75573-29-4 HCAPLUS

CN Silane, (3,3-dimethyl-1-butynyl)triethyl- (9CI) (CA INDEX NAME)



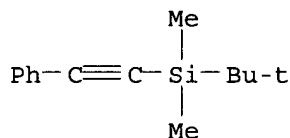
RN 79628-15-2 HCAPLUS

CN Silane, dimethylphenyl(phenylethynyl)- (9CI) (CA INDEX NAME)



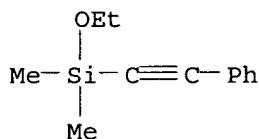
RN 85443-40-9 HCAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl(phenylethynyl)- (9CI) (CA INDEX NAME)



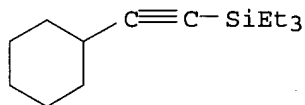
RN 146139-33-5 HCAPLUS

CN Silane, ethoxydimethyl(phenylethynyl)- (9CI) (CA INDEX NAME)



RN 148991-61-1 HCAPLUS

CN Silane, (cyclohexylethynyl)triethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 33 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:377084 HCAPLUS

DOCUMENT NUMBER: 125:58733

TITLE: Process for the preparation of 3-halo- or -pseudohalo-alkylsilane esters

INVENTOR(S): Kropfgans, Frank; Frings, Albert; Horn, Michael; Koetzsch, Hans-Joachim; Monkiewicz, Jaroslaw; Seiler, Claus-Dietrich; Srebny, Hans-Guenther; Standke, Burkhard

PATENT ASSIGNEE(S): Huels Aktiengesellschaft, Germany

SOURCE: Eur. Pat. Appl., 9 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

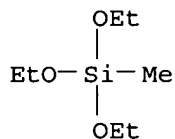
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

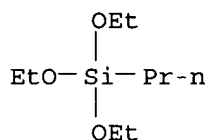
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 709392	A1	19960501	EP 1995-113741	19950901
EP 709392	B1	20010516		
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
DE 19534853	A1	19960502	DE 1995-19534853	19950920
CA 2161181	AA	19960426	CA 1995-2161181	19951023
JP 08208667	A2	19960813	JP 1995-275580	19951024
US 5616762	A	19970401	US 1995-548131	19951025
PRIORITY APPLN. INFO.:			DE 1994-4438031	A 19941025
			DE 1995-19534853	A 19950920
OTHER SOURCE(S): CASREACT 125:58733; MARPAT 125:58733				
AB	The preparation of title compds., XCR2R3CHR1CH2SiRn(OR4)3-n (R = C1-18 alkyl or cycloalkyl, halo; R1 = H, R; R2 = H, R, substituted aryl, halo; R3 = same or different R2; R3 = C1-10 alkyl, aliphatic ether containing group; X = F, Cl, Br, iodo, cyano, isocyanato, isothiocyanato, azido; n = 0-2) via iridium catalyzed hydrosilylation of XCR2R3CR1:CH2 with HSiRn(OR4)3-n is described. Thus, IrCl3 hydrate catalyzed hydrosilylation of allyl chloride with triethoxysilane in 3-chloropropyltriethoxysilane as reaction medium gave 86% 3-chloropropyltriethoxysilane.			
IC	ICM C07F007-18			
CC	29-6 (Organometallic and Organometalloidal Compounds)			
IT	78-10-4P, Tetraethoxysilane 2031-67-6P , Methyltriethoxysilane 2550-02-9P , Propyltriethoxysilane 177951-95-0P , Isobutyldiethoxymethylsilane			
	RL: BYP (Byproduct); PREP (Preparation) (preparation of)			
IT	5089-70-3P , 3-Chloropropyltriethoxysilane 24801-88-5P , 3-Isocyanatopropyltriethoxysilane 122055-02-1P , (3-Isothiocyanatopropyl)trimethoxysilane 177951-94-9P , (3-Chloroisobutyl)diethoxymethylsilane 177951-96-1P , Cyclopentylldiethoxy(3,3,3-trifluoropropyl)silane 177951-97-2P , 3-Bromopropyl(2-butoxyethoxy)dimethylsilane 177951-98-3P , (3,4-Dichloro-2-methylbutyl)ethyldimethoxysilane			
	RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)			
IT	12112-67-3 , Chloro(1,5-cyclooctadiene)iridium dimer 14996-61-3, Iridium trichloride hydrate 16941-92-7, Dihydrogen hexachloroiridate 51812-37-4 , Carbonylchlorobis(cyclooctadiene)iridium dimer			
	RL: CAT (Catalyst use) ; USES (Uses) (preparation of halo or pseudohalo substituted alkylsilane esters via iridium catalyzed hydrosilylation of unsatd. compds. with alkoxyasilanes)			
IT	57-06-7 106-95-6, Allyl bromide, reactions 107-05-1, Allyl chloride 563-47-3, Methallyl chloride 677-21-4, 3,3,3-Trifluoro-1-propene 998-30-1 , Triethoxysilane 1476-23-9, Allyl isocyanate 2031-62-1 , Methyltriethoxysilane 2487-90-3 , Trimethoxysilane 19753-84-5 , Ethyldimethoxysilane 53920-89-1 177951-92-7, Cyclopentylldiethoxysilane 177951-93-8 , (2-Butoxyethoxy)dimethylsilane			
	RL: RCT (Reactant) ; RACT (Reactant or reagent) (preparation of halo or pseudohalo substituted alkylsilane esters via iridium catalyzed hydrosilylation of unsatd. compds. with alkoxyasilanes)			
IT	2031-67-6P , Methyltriethoxysilane 2550-02-9P , Propyltriethoxysilane 177951-95-0P , Isobutyldiethoxymethylsilane			
	RL: BYP (Byproduct); PREP (Preparation) (preparation of)			
RN	2031-67-6 HCAPLUS			

CN Silane, triethoxymethyl- (8CI, 9CI) (CA INDEX NAME)



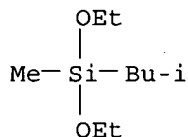
RN 2550-02-9 HCAPLUS

CN Silane, triethoxypropyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 177951-95-0 HCAPLUS

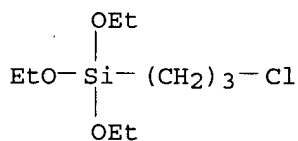
CN Silane, diethoxymethyl(2-methylpropyl)- (9CI) (CA INDEX NAME)



IT 5089-70-3P, 3-Chloropropyltriethoxysilane 24801-88-5P,
3-Isocyanatopropyltriethoxysilane 122055-02-1P,
(3-Isothiocyantopropyl)trimethoxysilane 177951-94-9P,
(3-Chloroisobutyl)diethoxymethylsilane 177951-96-1P,
Cyclopentyl-diethoxy(3,3,3-trifluoropropyl)silane 177951-97-2P,
3-Bromopropyl(2-butoxyethoxy)dimethylsilane 177951-98-3P,
(3,4-Dichloro-2-methylbutyl)ethyldimethoxysilane
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

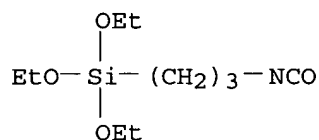
RN 5089-70-3 HCAPLUS

CN Silane, (3-chloropropyl)triethoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



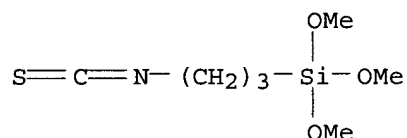
RN 24801-88-5 HCAPLUS

CN Silane, triethoxy(3-isocyanatopropyl)- (9CI) (CA INDEX NAME)



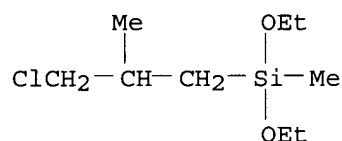
RN 122055-02-1 HCAPLUS

CN Silane, (3-isothiocyanatopropyl)trimethoxy- (9CI) (CA INDEX NAME)



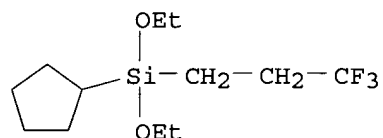
RN 177951-94-9 HCAPLUS

CN Silane, (3-chloro-2-methylpropyl)diethoxymethyl- (9CI) (CA INDEX NAME)



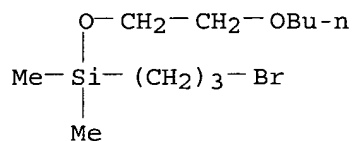
RN 177951-96-1 HCAPLUS

CN Silane, cyclopentyldiethoxy(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)



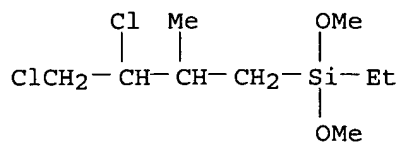
RN 177951-97-2 HCAPLUS

CN Silane, (3-bromopropyl)(2-butoxyethoxy)dimethyl- (9CI) (CA INDEX NAME)



RN 177951-98-3 HCAPLUS

CN Silane, (3,4-dichloro-2-methylbutyl)ethyldimethoxy- (9CI) (CA INDEX NAME)



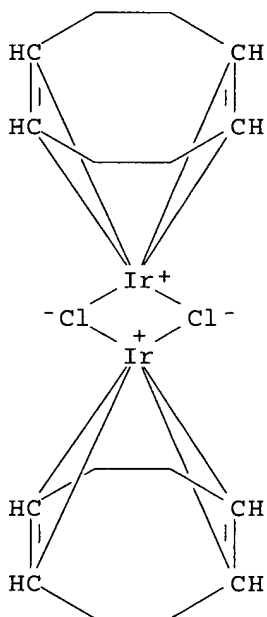
IT 12112-67-3, Chloro(1,5-cyclooctadiene)iridium dimer
 51812-37-4, Carbonylchlorobis(cyclooctadiene)iridium dimer

RL: CAT (Catalyst use); USES (Uses)

(preparation of halo or pseudohalo substituted alkylsilane esters via
 iridium catalyzed hydrosilylation of unsatd. compds. with
 alkoxyasilanes)

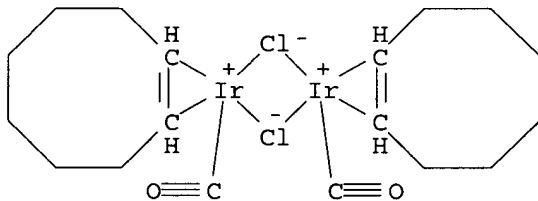
RN 12112-67-3 HCAPLUS

CN Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI)
 (CA INDEX NAME)



RN 51812-37-4 HCAPLUS

CN Iridium, dicarbonyldi-μ-chlorobis[(1,2-η)-cyclooctene]di- (9CI)
 (CA INDEX NAME)



IT 998-30-1, Triethoxysilane 2031-62-1,
 Methyldiethoxysilane 2487-90-3, Trimethoxysilane

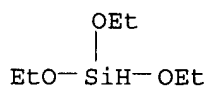
19753-84-5, Ethyldimethoxysilane 177951-93-8,
(2-Butoxyethoxy)dimethylsilane

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of halo or pseudohalo substituted alkylsilane esters via
iridium catalyzed hydrosilylation of unsatd. compds. with
alkoxysilanes)

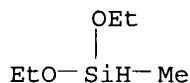
RN 998-30-1 HCAPLUS

CN Silane, triethoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)



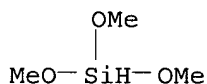
RN 2031-62-1 HCAPLUS

CN Silane, diethoxymethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



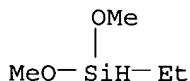
RN 2487-90-3 HCAPLUS

CN Silane, trimethoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



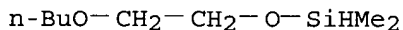
RN 19753-84-5 HCAPLUS

CN Silane, ethyldimethoxy- (8CI, 9CI) (CA INDEX NAME)



RN 177951-93-8 HCAPLUS

CN Silane, (2-butoxyethoxy)dimethyl- (9CI) (CA INDEX NAME)



L64 ANSWER 34 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:316883 HCAPLUS

DOCUMENT NUMBER: 122:160759

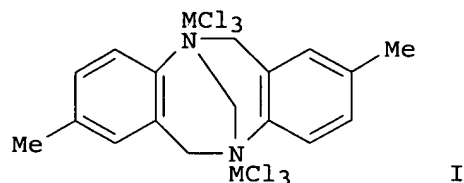
TITLE: Transition metal complexes of Troeger's base and their
catalytic activity for the hydrosilylation of alkynes

AUTHOR(S): Goldberg, Yuri; Alper, Howard

CORPORATE SOURCE: Department Chemistry, University Ottawa, Ottawa, ON,
K1N 6N5, Can.

SOURCE: Tetrahedron Letters (1995), 36(3), 369-72
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 122:160759
 GI



AB Rhodium(III) and iridium(III) complexes of Troger's base (TB), of structural type I (M = Rh, Ir), were prepared by treatment of TB with MCl₃. The rhodium complex readily catalyzed the hydrosilylation of alkynes with high regio- and stereoselectivity observed in some cases.

CC 29-6 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 78

IT 3412-58-6P 3412-59-7P 21209-32-5P
 42478-41-1P 61518-55-6P 64545-09-1P
 64545-10-4P 64788-84-7P 64788-85-8P
 75645-33-9P 76372-98-0P 109681-42-7P
 130613-30-8P 130613-31-9P 144967-38-4P
 160424-09-9P 160424-10-2P 161403-16-3P
 161403-17-4P 161403-18-5P 161403-19-6P
 161403-20-9P 161403-21-0P 161403-22-1P
 161403-23-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

IT 161377-10-2P 161377-11-3P 161444-29-7P 161444-30-0P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP
 (Preparation); USES (Uses)

(transition metal complexes of Troeger's base and catalytic activity
 for hydrosilylation of alkynes)

IT 536-74-3, Phenylacetylene 617-86-7, Triethylsilane 693-02-7,
 1-Hexyne 766-77-8, Dimethylphenylsilane 1066-35-9,
 Chlorodimethylsilane 6485-79-6, Triisopropylsilane
 10025-78-2, Trichlorosilane 14267-92-6 29681-57-0,
 tert-Butyldimethylsilane

RL: RCT (Reactant); RACT (Reactant or reagent)

(transition metal complexes of Troeger's base and catalytic activity
 for hydrosilylation of alkynes)

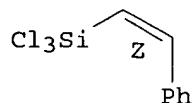
IT 3412-58-6P 3412-59-7P 21209-32-5P
 42478-41-1P 61518-55-6P 64545-09-1P
 64545-10-4P 64788-84-7P 64788-85-8P
 75645-33-9P 76372-98-0P 109681-42-7P
 130613-30-8P 130613-31-9P 144967-38-4P
 160424-09-9P 160424-10-2P 161403-16-3P
 161403-17-4P 161403-18-5P 161403-19-6P
 161403-20-9P 161403-21-0P 161403-22-1P
 161403-23-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 3412-58-6 HCAPLUS

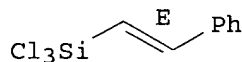
CN Silane, trichloro[(1Z)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



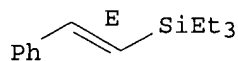
RN 3412-59-7 HCAPLUS
CN Silane, trichloro[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

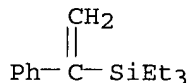


RN 21209-32-5 HCAPLUS
CN Silane, triethyl[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

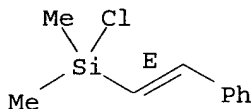


RN 42478-41-1 HCAPLUS
CN Silane, triethyl(1-phenylethenyl)- (9CI) (CA INDEX NAME)



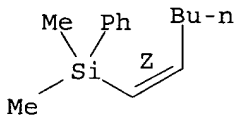
RN 61518-55-6 HCAPLUS
CN Silane, chlorodimethyl[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



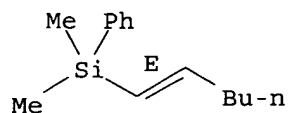
RN 64545-09-1 HCAPLUS
CN Silane, (1Z)-1-hexenyldimethylphenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 64545-10-4 HCAPLUS
CN Silane, (1E)-1-hexenyldimethylphenyl- (9CI) (CA INDEX NAME)

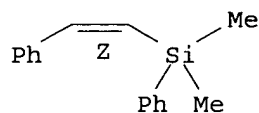
Double bond geometry as shown.



RN 64788-84-7 HCAPLUS

CN Silane, dimethylphenyl[(1Z)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

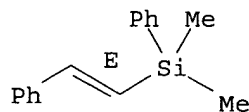
Double bond geometry as shown.



RN 64788-85-8 HCAPLUS

CN Silane, dimethylphenyl[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

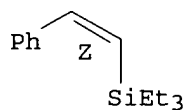
Double bond geometry as shown.



RN 75645-33-9 HCAPLUS

CN Silane, triethyl[(1Z)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

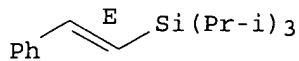
Double bond geometry as shown.



RN 76372-98-0 HCAPLUS

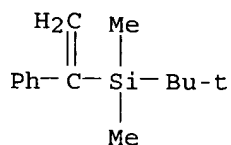
CN Silane, tris(1-methylethyl)(2-phenylethenyl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 109681-42-7 HCAPLUS

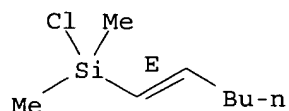
CN Silane, (1,1-dimethylethyl)dimethyl(1-phenylethenyl)- (9CI) (CA INDEX NAME)



RN 130613-30-8 HCAPLUS

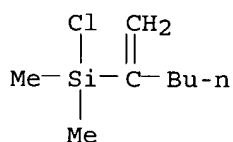
CN Silane, chloro-(1E)-1-hexenyldimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 130613-31-9 HCAPLUS

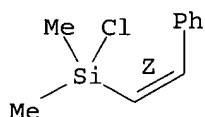
CN Silane, chlorodimethyl(1-methylenepentyl)- (9CI) (CA INDEX NAME)



RN 144967-38-4 HCAPLUS

CN Silane, chlorodimethyl[(1Z)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

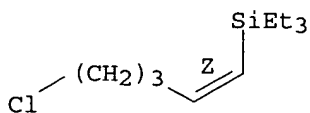
Double bond geometry as shown.



RN 160424-09-9 HCAPLUS

CN Silane, (5-chloro-1-pentenyl)triethyl-, (Z)- (9CI) (CA INDEX NAME)

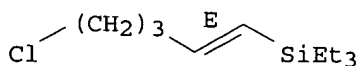
Double bond geometry as shown.



RN 160424-10-2 HCAPLUS

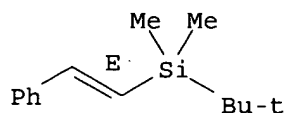
CN Silane, [(1E)-5-chloro-1-pentenyl]triethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

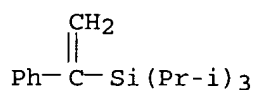


RN 161403-16-3 HCAPLUS
 CN Silane, (1,1-dimethylethyl)dimethyl[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

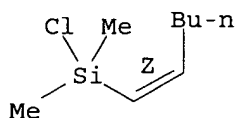


RN 161403-17-4 HCAPLUS
 CN Silane, tris(1-methylethyl)(1-phenylethenyl)- (9CI) (CA INDEX NAME)



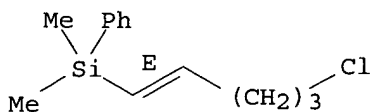
RN 161403-18-5 HCAPLUS
 CN Silane, chloro-1-hexenyldimethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



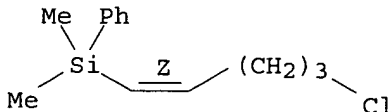
RN 161403-19-6 HCAPLUS
 CN Silane, [(1E)-5-chloro-1-pentenyl]dimethylphenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



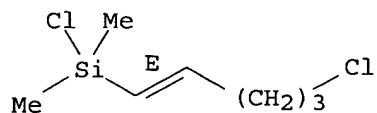
RN 161403-20-9 HCAPLUS
 CN Silane, (5-chloro-1-pentenyl)dimethylphenyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 161403-21-0 HCAPLUS
 CN Silane, chloro(5-chloro-1-pentenyl)dimethyl-, (E)- (9CI) (CA INDEX NAME)

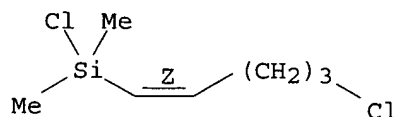
Double bond geometry as shown.



RN 161403-22-1 HCAPLUS

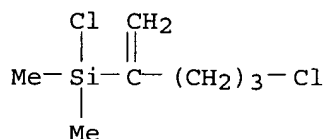
CN Silane, chloro(5-chloro-1-pentenyl)dimethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 161403-23-2 HCAPLUS

CN Silane, chloro(4-chloro-1-methylenebutyl)dimethyl- (9CI) (CA INDEX NAME)



IT 161377-11-3P

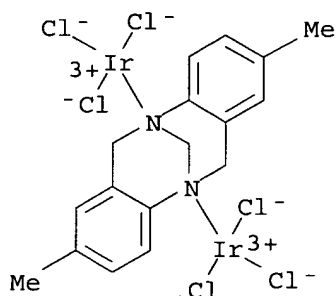
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP

(Preparation); USES (Uses)

(transition metal complexes of Troeger's base and catalytic activity for hydrosilylation of alkynes)

RN 161377-11-3 HCAPLUS

CN Iridium, hexachloro[μ-(2,8-dimethyl-6H,12H-5,11-methanodibenzo[b,f][1,5]diazocine-N5:N11)]di- (9CI) (CA INDEX NAME)



IT 617-86-7, Triethylsilane 1066-35-9, Chlorodimethylsilane

6485-79-6, Triisopropylsilane 10025-78-2,

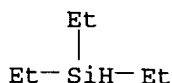
Trichlorosilane 29681-57-0, tert-Butyldimethylsilane

RL: RCT (Reactant); RACT (Reactant or reagent)

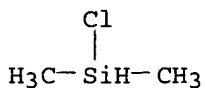
(transition metal complexes of Troeger's base and catalytic activity for hydrosilylation of alkynes)

RN 617-86-7 HCAPLUS

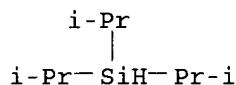
CN Silane, triethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



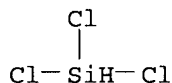
RN 1066-35-9 HCAPLUS
CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



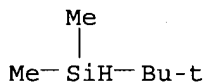
RN 6485-79-6 HCAPLUS
CN Silane, tris(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 10025-78-2 HCAPLUS
CN Silane, trichloro- (8CI, 9CI) (CA INDEX NAME)



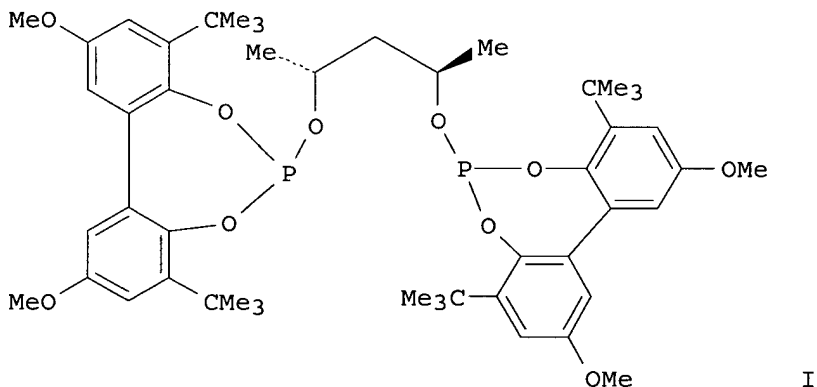
RN 29681-57-0 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



L64 ANSWER 35 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:229480 HCAPLUS
DOCUMENT NUMBER: 122:186609
TITLE: Asymmetric syntheses using optically active
metal-ligand complex catalysts
INVENTOR(S): Babin, James E.; Whiteker, Gregory T.
PATENT ASSIGNEE(S): Union Carbide Chemicals and Plastics Technology Corp.,
USA
SOURCE: U.S., 23 pp. Cont.-in-part of U.S. Ser. No. 748,112.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 5360938	A	19941101	US 1992-911518	19920716
IL 102873	A1	20010520	IL 1992-102873	19920819
ZA 9206289	A	19930303	ZA 1992-6289	19920820
WO 9303839	A1	19930304	WO 1992-US6808	19920820
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MG, MN, MW, NO, PL, RO, RU, SD				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9225077	A1	19930316	AU 1992-25077	19920820
CN 1071431	A	19930428	CN 1992-110864	19920820
CN 1038938	B	19980701		
EP 600020	A1	19940608	EP 1992-919034	19920820
EP 600020	B1	19960131		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, SE				
IN 174153	A	19940924	IN 1992-MA516	19920820
BR 9206391	A	19950301	BR 1992-6391	19920820
AT 133584	E	19960215	AT 1992-919034	19920820
ES 2085644	T3	19960601	ES 1992-919034	19920820
CA 2116098	C	19980120	CA 1992-2116098	19920820
KR 136357	B1	19980425	KR 1994-700550	19940221
IN 178002	A	19970301	IN 1994-MA313	19940420
US 5491266	A	19960213	US 1994-262508	19940620
PRIORITY APPLN. INFO.:				B2 19910821
				A2 19910821
				A 19920716
				A1 19920820
				A 19920820
OTHER SOURCE(S):				MARPAT 122:186609
GI				



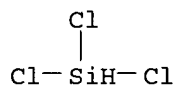
AB This invention relates to asym. syntheses in which a prochiral or chiral compound is contacted in the presence of an optically active metal-ligand complex catalyst to produce an optically active product. Thus, e.g., asym. hydroformylation of styrene with a catalyst solution containing rhodium dicarbonyl acetylacetonate and ligand I afforded an isomer ratio of 12.4:1 (2-phenylpropionaldehyde:hydrocinnamaldehyde); oxidation of the product aldehydes afforded an 80:20 ratio of the S and R enantiomers of 2-phenylpropionic acid.

IC ICM C07C045-00
INCL 568449000

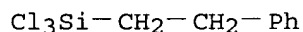
- CC 21-2 (General Organic Chemistry)
- IT 1295-35-8, Bis(1,5-cyclooctadiene)nickel(0) 7439-88-5D,
Iridium, optically active ligand complexes 7439-89-6D, Iron, optically
active ligand complexes 7440-02-0D, Nickel, optically active ligand
complexes 7440-04-2D, Osmium, optically active ligand complexes
7440-05-3D, Palladium, optically active ligand complexes 7440-06-4D,
Platinum, optically active ligand complexes 7440-16-6D, Rhodium,
optically active ligand complexes 7440-18-8D, Ruthenium, optically
active ligand complexes 7440-48-4D, Cobalt, optically active ligand
complexes 7758-89-6, Copper(I) chloride 12111-11-4,
Bicyclo[2.2.1]hepta-2,5-dieneiridium(I) chloride dimer
14284-93-6 14874-82-9, Rhodium dicarbonyl acetylacetonate 38816-56-7,
Bis(bicyclo[2.2.1]hepta-2,5-diene)rhodium(I) hexafluorophosphate
60576-58-1, Bis(bicyclo[2.2.1]hepta-2,5-diene)rhodium(I)
perchlorate 90243-59-7, cis-Dichlorobis(acetonitrile)palladium(II)
RL: CAT (Catalyst use); USES (Uses)
(asym. synthesis using optically active metal-ligand complex catalysts)
- IT 97-65-4, Itaconic Acid, reactions 98-83-9, α -Methylstyrene,
reactions 98-86-2, Acetophenone, reactions 100-42-5, Styrene,
reactions 100-52-7, Benzaldehyde, reactions 108-05-4, Vinyl Acetate,
reactions 128-37-0, 2,6-Di-tert-butyl-4-methylphenol, reactions
498-66-8, Norbornene 592-41-6, 1-Hexene, reactions 1079-66-9,
Chlorodiphenylphosphine 10025-78-2, Trichlorosilane 16611-68-0
18531-94-7 18531-99-2, (S)-1,1'-Bi-2-naphthol 31469-15-5, Methyl
trimethylsilyl dimethylketene acetal 42075-32-1, (2R,4R)-Pentanediol
63444-51-9, 6-Methoxy-2-vinylnaphthalene 63444-56-4, p-Isobutylstyrene
71941-98-5 72345-23-4, (2S,4S)-Pentanediol 73346-74-4,
(-)-2,3-O-Isopropylidene-D-threitol 82017-87-6 108609-95-6
134170-23-3 137156-22-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. synthesis using optically active metal-ligand complex catalysts)
- IT 940-41-0P, 2-Trichlorosilyl ethylbenzene 32305-59-2P
33530-47-1P, (S)-2-Phenylpropionaldehyde 38235-74-4P,
(R)-2-Phenylpropionaldehyde 56800-48-7P 110773-62-1P 114937-27-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(asym. synthesis using optically active metal-ligand complex catalysts)
- IT 60-12-8P, 2-Phenylethanol 111-71-7P, n-Heptanal 645-59-0P,
Hydrocinnamonitrile 939-90-2P 1445-91-6P 1517-69-7P 2174-58-5P
2234-26-6P, 2-Norbornanecarbonitrile 3641-51-8P 7782-24-3P,
(S)-2-Phenylpropionic acid 7782-26-5P, (R)-2-Phenylpropionic acid
13340-46-0P, 2-Triethoxysilyl ethylbenzene 22204-53-1P
23020-18-0P 42307-58-4P, (R)-3-Phenylbutyraldehyde 42412-76-0P
48126-51-8P 51146-56-6P 53531-19-4P, (S)-3-Phenylbutyraldehyde
55630-27-8P 60933-33-7P 66875-69-2P, (R)- α -Acetoxypropanal
66875-70-5P, (S)- α -Acetoxypropanal 66875-71-6P,
(S)-2-Methylhexanal 79201-73-3P 104418-69-1P 110849-52-0P
132151-88-3P, (R)-2-Methylhexanal 159909-89-4P
159909-90-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis using optically active metal-ligand complex catalysts)
- IT 12111-11-4, Bicyclo[2.2.1]hepta-2,5-dieneiridium(I)
chloride dimer
RL: CAT (Catalyst use); USES (Uses)
(asym. synthesis using optically active metal-ligand complex catalysts)
- RN 12111-11-4 HCAPLUS
- CN Iridium, bis[(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene]di- μ -
chlorodi- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

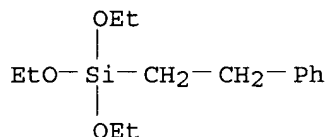
IT 10025-78-2, Trichlorosilane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (asym. synthesis using optically active metal-ligand complex catalysts)
 RN 10025-78-2 HCAPLUS
 CN Silane, trichloro- (8CI, 9CI) (CA INDEX NAME)



IT 940-41-0P, 2-Trichlorosilylethylbenzene
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (asym. synthesis using optically active metal-ligand complex catalysts)
 RN 940-41-0 HCAPLUS
 CN Silane, trichloro(2-phenylethyl)- (9CI) (CA INDEX NAME)

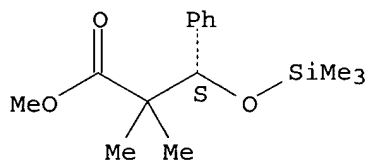


IT 13340-46-0P, 2-Triethoxysilylethylbenzene 159909-89-4P
 159909-90-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (asym. synthesis using optically active metal-ligand complex catalysts)
 RN 13340-46-0 HCAPLUS
 CN Silane, triethoxy(2-phenylethyl)- (9CI) (CA INDEX NAME)



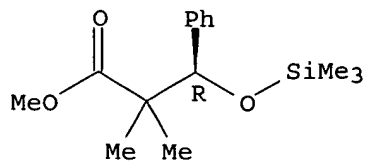
RN 159909-89-4 HCAPLUS
 CN Benzenepropanoic acid, α,α -dimethyl- β -
 [(trimethylsilyl)oxy]-, methyl ester, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159909-90-7 HCAPLUS
 CN Benzenepropanoic acid, α,α -dimethyl- β -
 [(trimethylsilyl)oxy]-, methyl ester, (β R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L64 ANSWER 36 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:651413 HCAPLUS

DOCUMENT NUMBER: 117:251413

TITLE: Conversion of **alkenes** to enol silyl ethers of acylsilanes by iridium-catalyzed reaction with a hydrosilane and carbon monoxide

AUTHOR(S): Chatani, Naoto; Ikeda, Shinichi; Ohe, Kouichi; Murai, Shinji

CORPORATE SOURCE: Fac. Eng., Osaka Univ., Suita, 565, Japan

SOURCE: Journal of the American Chemical Society (1992), 114(24), 9710-11

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:251413

AB The reaction of **alkenes**, e.g., RCH:CH₂ (R = Bu, cyclohexyl, Me₃C, etc.; 5-10 equiv, 14 examples) with a hydrosilane (1 equiv, HSiEt₂Me, HSiEt₃, HSiPhMe₂) and CO (50 atm) in the presence of an iridium complex (0.02 equiv, [IrCl(CO)₃]_n, Ir₄(CO)₁₂) at 140° in benzene resulted in the incorporation of CO to give an E/Z mixture of 1-silyl enol silyl ethers, RCH₂CH:C(SiR₁₃)(OSiR₁₃) (II) in 45-85% yields. II can be easily hydrolyzed to acylsilanes, e.g. BuCH₂CH₂COSiEt₂Me, (acetone/HCl (0.2 M) = 4/1 at 25°). The overall transformation is a novel, unique method for the preparation of acylsilanes from **alkenes**.

CC 29-6 (Organometallic and Organometalloidal Compounds)

ST **alkene** hydrosilylation iridium catalyzed carbon monoxide; regiochem iridium catalyzed hydrosilylation **alkene**; enol silyl ether prepn hydrolysis; acylsilane

IT **Alkenes**, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrosilylation of, in presence of carbon monoxide, iridium-catalyzed, enol silyl ethers by)

IT Hydrosilylation catalysts

(iridium complexes, for **alkenes** in presence of carbon monoxide, enol silyl ethers by)

IT Hydrosilylation

(of **alkenes** in presence of carbon monoxide, enol silyl ethers by)

IT Regiochemistry

(of hydrosilylation of **alkenes** with hydrosilanes in presence of carbon monoxide, enol silyl ethers by)

IT Ethers, preparation

RL: SPN (Synthetic preparation); PREP (Preparation)

(enol, silyl, preparation of, by iridium-catalyzed hydrosilylation of **alkenes** in presence of carbon monoxide)

IT 18827-81-1 32594-40-4

RL: CAT (Catalyst use); USES (Uses)

(catalysts, for iridium-catalyzed hydrosilylation of **alkenes** with hydrosilanes in presence of carbon monoxide)

IT 617-86-7, Triethylsilane 760-32-7, Methyl-diethylsilane

766-77-8, Dimethylphenylsilane

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrosilylation by, of **alkenes** in presence of carbon monoxide, iridium-catalyzed, enol silyl ether by)

IT 144542-05-2P 144542-06-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of, acylsilane by)

IT 144542-07-4P 144542-08-5P 144542-09-6P

144542-10-9P 144542-11-0P 144542-12-1P

144542-13-2P 144542-14-3P 144542-15-4P

144542-16-5P 144542-17-6P 144542-18-7P

144542-19-8P 144542-20-1P 144542-21-2P

144542-22-3P 144542-23-4P 144542-24-5P

144542-25-6P 144542-26-7P 144542-27-8P

144542-28-9P 144542-29-0P 144542-30-3P

144542-31-4P 144542-32-5P 144542-33-6P

144542-34-7P 144542-35-8P 144564-72-7P

144564-73-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

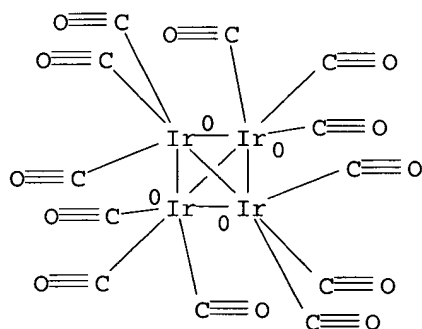
IT 18827-81-1

RL: CAT (Catalyst use); USES (Uses)

(catalysts, for iridium-catalyzed hydrosilylation of **alkenes** with hydrosilanes in presence of carbon monoxide)

RN 18827-81-1 HCAPLUS

CN Iridium, dodecacarbonyltetra-, tetrahedro (9CI) (CA INDEX NAME)



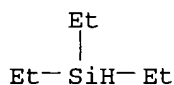
IT 617-86-7, Triethylsilane 760-32-7, Methyl-diethylsilane

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrosilylation by, of **alkenes** in presence of carbon monoxide, iridium-catalyzed, enol silyl ether by)

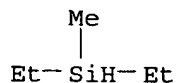
RN 617-86-7 HCAPLUS

CN Silane, triethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 760-32-7 HCAPLUS

CN Silane, diethylmethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



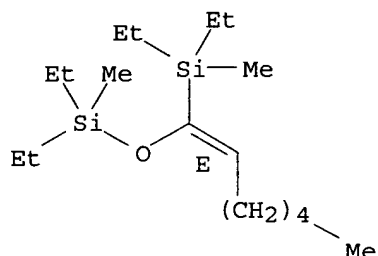
IT 144542-05-2P 144542-06-3P

RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**
(**Preparation**); RACT (Reactant or reagent)
(preparation and hydrolysis of, acylsilane by)

RN 144542-05-2 HCAPLUS

CN Silane, [[1-(diethylmethylsilyl)-1-heptenyl]oxy]diethylmethyl-, (E)- (9CI)
(CA INDEX NAME)

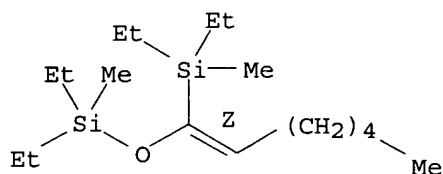
Double bond geometry as shown.



RN 144542-06-3 HCAPLUS

CN Silane, [[1-(diethylmethylsilyl)-1-heptenyl]oxy]diethylmethyl-, (Z)- (9CI)
(CA INDEX NAME)

Double bond geometry as shown.



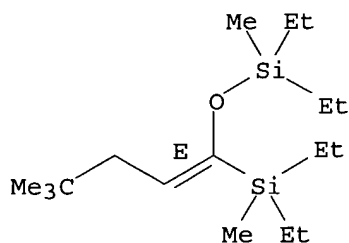
IT 144542-07-4P 144542-08-5P 144542-09-6P
144542-10-9P 144542-11-0P 144542-12-1P
144542-13-2P 144542-14-3P 144542-15-4P
144542-16-5P 144542-17-6P 144542-18-7P
144542-19-8P 144542-20-1P 144542-21-2P
144542-22-3P 144542-23-4P 144542-24-5P
144542-25-6P 144542-26-7P 144542-27-8P
144542-28-9P 144542-29-0P 144542-30-3P
144542-31-4P 144542-32-5P 144542-33-6P
144542-34-7P 144542-35-8P 144564-72-7P
144564-73-8P

RL: SPN (Synthetic preparation); **PREP** (**Preparation**)
(preparation of)

RN 144542-07-4 HCAPLUS

CN Silane, [[1-(diethylmethylsilyl)-4,4-dimethyl-1-pentenyl]oxy]diethylmethyl-, (E)- (9CI) (CA INDEX NAME)

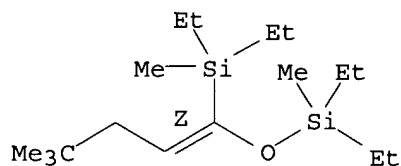
Double bond geometry as shown.



RN 144542-08-5 HCAPLUS

CN Silane, [[1-(diethylmethylsilyl)-4,4-dimethyl-1-pentenyl]oxy]diethylmethyl-, (Z)- (9CI) (CA INDEX NAME)

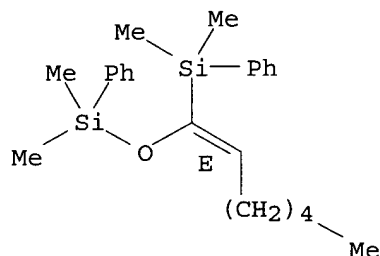
Double bond geometry as shown.



RN 144542-09-6 HCAPLUS

CN Silane, [[1-(dimethylphenylsilyl)-1-heptenyl]oxy]dimethylphenyl-, (E)- (9CI) (CA INDEX NAME)

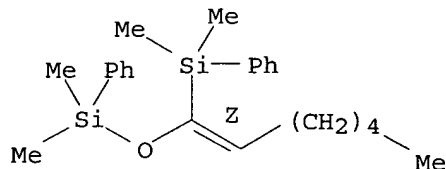
Double bond geometry as shown.



RN 144542-10-9 HCAPLUS

CN Silane, [[1-(dimethylphenylsilyl)-1-heptenyl]oxy]dimethylphenyl-, (Z)- (9CI) (CA INDEX NAME)

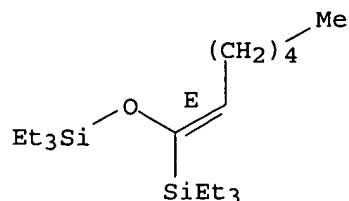
Double bond geometry as shown.



RN 144542-11-0 HCAPLUS

CN Silane, triethyl[[1-(triethylsilyl)-1-heptenyl]oxy]-, (E)- (9CI) (CA INDEX NAME)

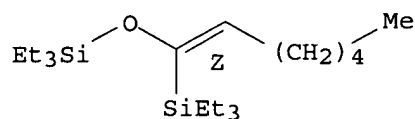
Double bond geometry as shown.



RN 144542-12-1 HCAPLUS

CN Silane, triethyl[[1-(triethylsilyl)-1-heptenyl]oxy]-, (Z)- (9CI) (CA INDEX NAME)

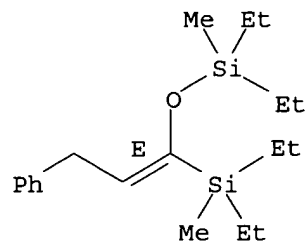
Double bond geometry as shown.



RN 144542-13-2 HCAPLUS

CN Silane, [1-[(diethylmethylsilyl)oxy]-3-phenyl-1-propenyl]diethylmethyl-, (E)- (9CI) (CA INDEX NAME)

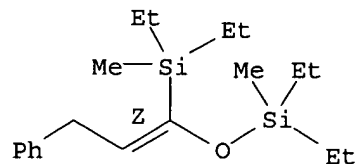
Double bond geometry as shown.



RN 144542-14-3 HCAPLUS

CN Silane, [1-[(diethylmethylsilyl)oxy]-3-phenyl-1-propenyl]diethylmethyl-, (Z)- (9CI) (CA INDEX NAME)

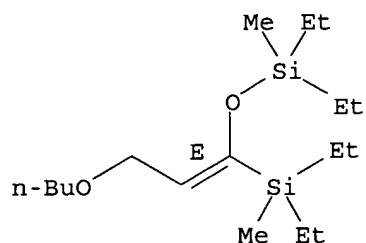
Double bond geometry as shown.



RN 144542-15-4 HCAPLUS

CN Silane, [3-butoxy-1-[(diethylmethylsilyl)oxy]-1-propenyl]diethylmethyl-, (E)- (9CI) (CA INDEX NAME)

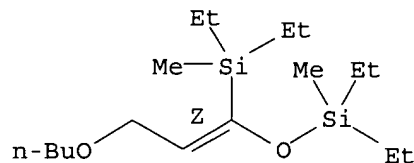
Double bond geometry as shown.



RN 144542-16-5 HCAPLUS

CN Silane, [3-butoxy-1-[(diethylmethylsilyl)oxy]-1-propenyl]diethylmethyl-, (Z)- (9CI) (CA INDEX NAME)

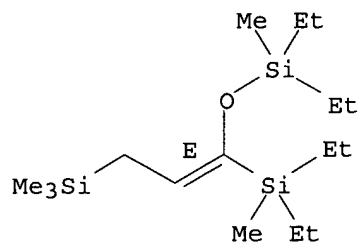
Double bond geometry as shown.



RN 144542-17-6 HCAPLUS

CN Silane, [3-(diethylmethylsilyl)-3-[(diethylmethylsilyl)oxy]-2-propenyl]trimethyl-, (E)- (9CI) (CA INDEX NAME)

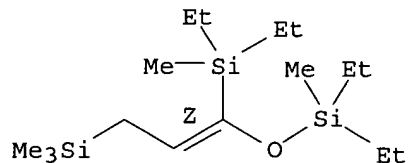
Double bond geometry as shown.



RN 144542-18-7 HCAPLUS

CN Silane, [3-(diethylmethylsilyl)-3-[(diethylmethylsilyl)oxy]-2-propenyl]trimethyl-, (Z)- (9CI) (CA INDEX NAME)

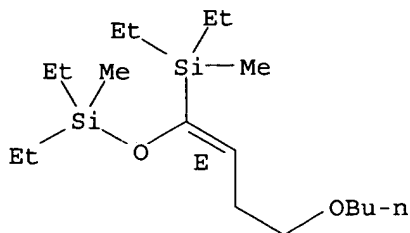
Double bond geometry as shown.



RN 144542-19-8 HCAPLUS

CN Silane, [[4-butoxy-1-(diethylmethylsilyl)-1-butenyl]oxy]diethylmethyl-, (E)- (9CI) (CA INDEX NAME)

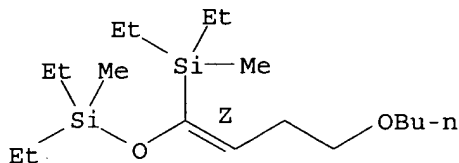
Double bond geometry as shown.



RN 144542-20-1 HCAPLUS

CN Silane, [[4-butoxy-1-(diethylmethylsilyl)-1-butenyl]oxy]diethylmethyl-, (Z)- (9CI) (CA INDEX NAME)

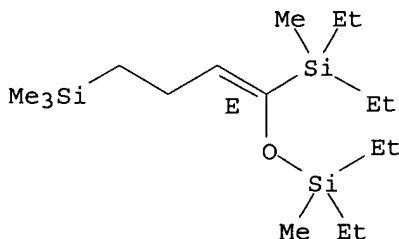
Double bond geometry as shown.



RN 144542-21-2 HCAPLUS

CN Silane, [4-(diethylmethylsilyl)-4-[(diethylmethylsilyl)oxy]-3-butenyl]trimethyl-, (E)- (9CI) (CA INDEX NAME)

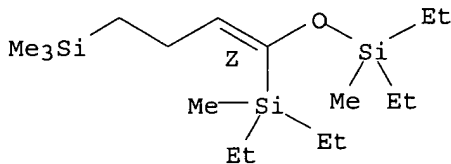
Double bond geometry as shown.



RN 144542-22-3 HCAPLUS

CN Silane, [4-(diethylmethylsilyl)-4-[(diethylmethylsilyl)oxy]-3-butenyl]trimethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

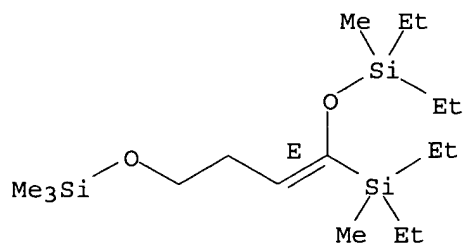


RN 144542-23-4 HCAPLUS

CN 3,8-Dioxa-2,9-disilaundec-6-ene, 7-(diethylmethylsilyl)-9-ethyl-2,2,9-

trimethyl-, (E)- (9CI) (CA INDEX NAME)

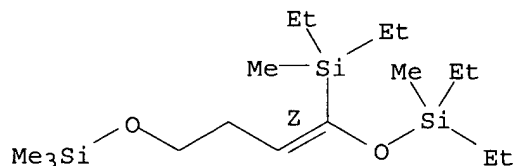
Double bond geometry as shown.



RN 144542-24-5 HCAPLUS

CN 3,8-Dioxa-2,9-disilaundec-6-ene, 7-(diethylmethylsilyl)-9-ethyl-2,2,9-trimethyl-, (Z)- (9CI) (CA INDEX NAME)

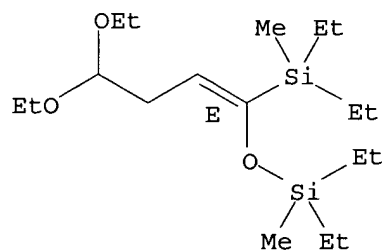
Double bond geometry as shown.



RN 144542-25-6 HCAPLUS

CN Silane, [[1-(diethylmethylsilyl)-4,4-diethoxy-1-butenyl]oxy]diethylmethyl-, (E)- (9CI) (CA INDEX NAME)

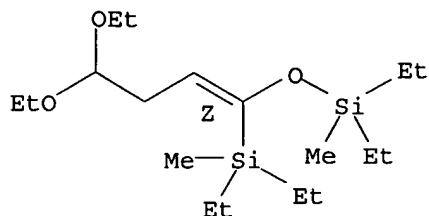
Double bond geometry as shown.



RN 144542-26-7 HCAPLUS

CN Silane, [[1-(diethylmethylsilyl)-4,4-diethoxy-1-butenyl]oxy]diethylmethyl-, (Z)- (9CI) (CA INDEX NAME)

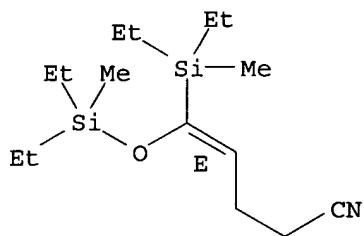
Double bond geometry as shown.



RN 144542-27-8 HCAPLUS

CN 4-Pentenitrile, 5-(diethylmethoxysilyl)-5-[(diethylmethoxysilyl)oxy]-,
(E)- (9CI) (CA INDEX NAME)

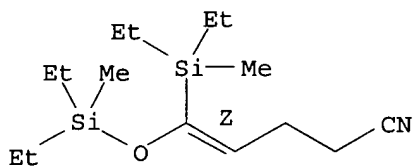
Double bond geometry as shown.



RN 144542-28-9 HCAPLUS

CN 4-Pentenitrile, 5-(diethylmethoxysilyl)-5-[(diethylmethoxysilyl)oxy]-,
(Z)- (9CI) (CA INDEX NAME)

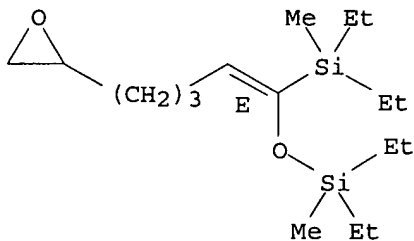
Double bond geometry as shown.



RN 144542-29-0 HCAPLUS

CN Silane, [[1-(diethylmethoxysilyl)-5-oxiranyl-1-pentenyl]oxy]diethylmethyl-,
(E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

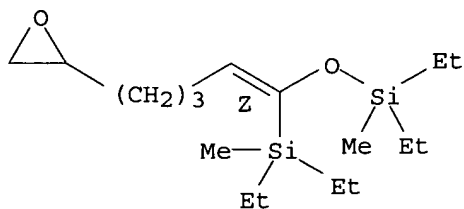


RN 144542-30-3 HCAPLUS

CN Silane, [[1-(diethylmethoxysilyl)-5-oxiranyl-1-pentenyl]oxy]diethylmethyl-,

(Z) - (9CI) (CA INDEX NAME)

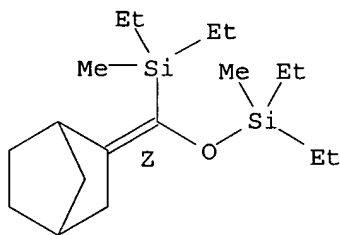
Double bond geometry as shown.



RN 144542-31-4 HCAPLUS

CN Silane, [bicyclo[2.2.1]hept-2-ylidene(diethylmethylsilyl)methoxy]diethylmethyl-, (Z) - (9CI) (CA INDEX NAME)

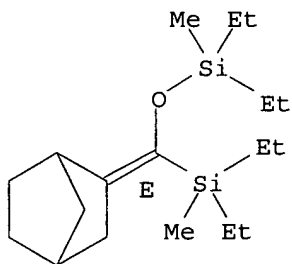
Double bond geometry as shown.



RN 144542-32-5 HCAPLUS

CN Silane, [bicyclo[2.2.1]hept-2-ylidene(diethylmethylsilyl)methoxy]diethylmethyl-, (E) - (9CI) (CA INDEX NAME)

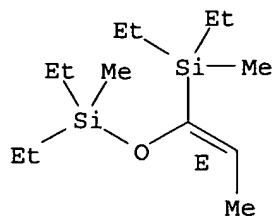
Double bond geometry as shown.



RN 144542-33-6 HCAPLUS

CN Silane, [[1-(diethylmethylsilyl)-1-propenyl]oxy]diethylmethyl-, (E) - (9CI) (CA INDEX NAME)

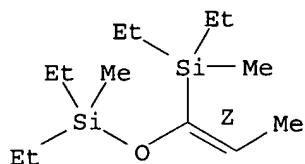
Double bond geometry as shown.



RN 144542-34-7 HCAPLUS

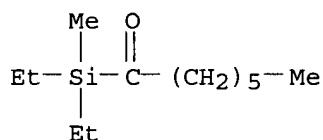
CN Silane, [[1-(diethylmethylsilyl)-1-propenyl]oxy]diethylmethyl-, (Z)- (9CI)
(CA INDEX NAME)

Double bond geometry as shown.



RN 144542-35-8 HCAPLUS

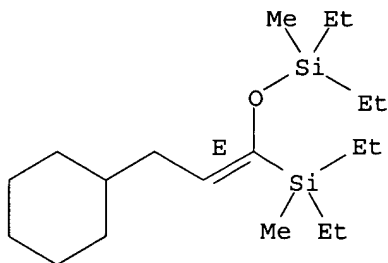
CN Silane, diethylmethyl(1-oxoheptyl)- (9CI) (CA INDEX NAME)



RN 144564-72-7 HCAPLUS

CN Silane, [3-cyclohexyl-1-[(diethylmethylsilyl)oxy]-1-propenyl]diethylmethyl-, (E)- (9CI) (CA INDEX NAME)

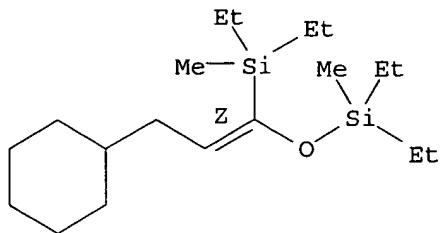
Double bond geometry as shown.



RN 144564-73-8 HCAPLUS

CN Silane, [3-cyclohexyl-1-[(diethylmethylsilyl)oxy]-1-propenyl]diethylmethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L64 ANSWER 37 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1987:496882 HCAPLUS
 DOCUMENT NUMBER: 107:96882
 TITLE: Novel process for the preparation of
 halopropyltrialkoxysilanes and
 halopropylalkylalkoxysilanes
 INVENTOR(S): Quirk, Jennifer M.; Kanner, Bernard
 PATENT ASSIGNEE(S): Union Carbide Corp., USA
 SOURCE: U.S., 5 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4658050	A	19870414	US 1986-846176	19860331
CA 1307287	A1	19920908	CA 1986-524638	19861205
EP 239677	A2	19871007	EP 1986-117784	19861219
EP 239677	A3	19880720		
EP 239677	B1	19900131		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 62230794	A2	19871009	JP 1986-301825	19861219
JP 02057076	B4	19901203		
AT 49974	E	19900215	AT 1986-117784	19861219
PRIORITY APPLN. INFO.:			US 1986-846176	A 19860331
			EP 1986-117784	A 19861219

AB XCH₂CHR₂CH₂SiR_n(OR₁)_{3-n} (R,R₁ = C₁-6 alkyl; R₂ = H, C₁-6 alkyl; X = Cl, Br, iodide; n = 0-2) are prepared by hydrosilylation of allylic halides in the presence of [Ir(L)X]₂ catalysts [L = (cyclo)diene]. A mixture of HSi(OEt)₃ 1, allyl chloride 0.5, and xylene 0.5 g was heated at 80° for 4 h in the presence of 0.19 mg [Ir(COD)Cl]₂ (COD = 1,5-cyclooctadiene) to give 75% ClCH₂CH₂CH₂Si(OEt)₃.

IC ICM C07F007-08
 ICS C07F007-18

INCL 556479000

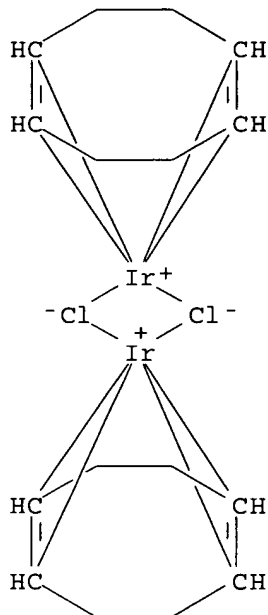
CC 29-6 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 67

IT Hydrosilylation catalysts
 (iridium cycloalkadiene halide dimers, for allylic halides)

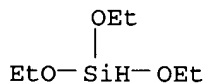
IT 12112-67-3
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst, for hydrosilylation of allyl chloride)

IT 998-30-1, Triethoxysilane 2031-62-1,
 Methyldiethoxysilane 2487-90-3, Trimethoxysilane
 6675-79-2, Triisopropoxysilane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrosilylation by, of allyl chloride)

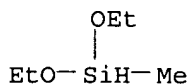
IT 2530-87-2P, 3-Chloropropyltrimethoxysilane 5089-70-3P,
 3-Chloropropyltriethoxysilane 13501-76-3P, 3-
 Chloropropylmethyldiethoxysilane 61214-14-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by hydrosilylation of allyl chloride)
 IT 12112-67-3
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst, for hydrosilylation of allyl chloride)
 RN 12112-67-3 HCAPLUS
 CN Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di- (9CI)
 (CA INDEX NAME)



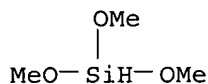
IT 998-30-1, Triethoxysilane 2031-62-1,
 Methyldiethoxysilane 2487-90-3, Trimethoxysilane
 6675-79-2, Triisopropoxysilane
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrosilylation by, of allyl chloride)
 RN 998-30-1 HCAPLUS
 CN Silane, triethoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)



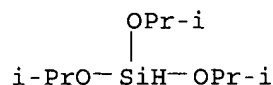
RN 2031-62-1 HCAPLUS
 CN Silane, diethoxymethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



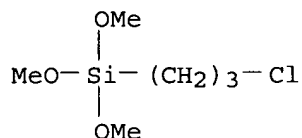
RN 2487-90-3 HCAPLUS
 CN Silane, trimethoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



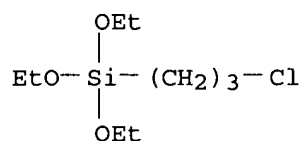
RN 6675-79-2 HCAPLUS
 CN Silane, tris(1-methylethoxy)- (9CI) (CA INDEX NAME)



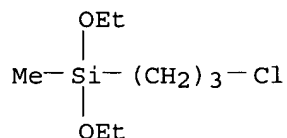
IT 2530-87-2P, 3-Chloropropyltrimethoxysilane 5089-70-3P,
 3-Chloropropyltriethoxysilane 13501-76-3P, 3-
 Chloropropylmethyldiethoxysilane 61214-14-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by hydrosilylation of allyl chloride)
 RN 2530-87-2 HCAPLUS
 CN Silane, (3-chloropropyl)trimethoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



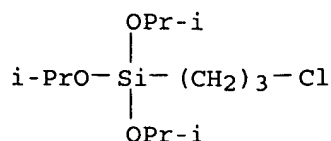
RN 5089-70-3 HCAPLUS
 CN Silane, (3-chloropropyl)triethoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 13501-76-3 HCAPLUS
 CN Silane, (3-chloropropyl)diethoxymethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



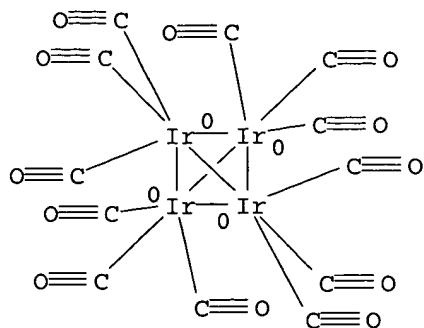
RN 61214-14-0 HCAPLUS
 CN Silane, (3-chloropropyl)tris(1-methylethoxy)- (9CI) (CA INDEX NAME)



L64 ANSWER 38 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1982:563243 HCAPLUS
 DOCUMENT NUMBER: 97:163243
 TITLE: Photoactivated catalytic hydrosilylation of carbonyl compounds
 INVENTOR(S): Yates, Ronald L.
 PATENT ASSIGNEE(S): Dow Chemical Co., USA
 SOURCE: U.S., 8 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4332654	A	19820601	US 1981-284034	19810717
US 4383120	A	19830510	US 1981-320237	19811112
PRIORITY APPLN. INFO.: MARPAT 97:163243			US 1981-284034	A2 19810717

OTHER SOURCE(S):
 AB Photohydrosilylation of acetone with HSiEt₃ gave Me₂CHOSiEt₃. Transition metal carbonyls, Re₂(CO)₁₀, Ir₄(CO)₁₂, Os₃(CO)₁₂, Ru₃(CO)₁₂, LIr(CO)₂ (L = acetylacetonate), Fe₃(CO)₁₂, Co₂(CO)₈, Cr(CO)₆, Rh₆(CO)₁₆, Co₂(CO)₆(PPh₃)₂, Co₄(CO)₁₂, and Fe₂(CO)₉, were used as catalysts. Ac(CH₂)₄Me, cycloheptanone, and PrCHO were also photohydrosilylated with HSiEt₃.
 IC C07F007-18
 INCL 204158000R
 CC 29-6 (Organometallic and Organometalloidal Compounds)
 IT 10210-68-1 13007-92-6 14023-80-4 14285-68-8 15243-33-1
 15321-51-4 15696-40-9 17685-52-8 17786-31-1 **18827-81-1**
 24212-54-2 28407-51-4
 RL: **CAT (Catalyst use)**; USES (Uses)
 (catalyst, for photohydrosilylation of carbonyl compds.)
 IT **617-86-7**
 RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
 (photohydrosilylation of carbonyl compds. with, catalysts for)
 IT **1571-45-5P**
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
 (preparation and hydrolysis of)
 IT **2751-87-3P 51276-59-6P** 83276-09-9P
 RL: SPN (Synthetic preparation); **PREP (Preparation)**
 (preparation of)
 IT **18827-81-1**
 RL: **CAT (Catalyst use)**; USES (Uses)
 (catalyst, for photohydrosilylation of carbonyl compds.)
 RN 18827-81-1 HCAPLUS
 CN Iridium, dodecacarbonyltetra-, tetrahedro (9CI) (CA INDEX NAME)



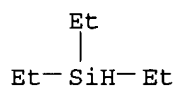
IT 617-86-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(photohydrosilylation of carbonyl compds. with, catalysts for)

RN 617-86-7 HCAPLUS

CN Silane, triethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT 1571-45-5P

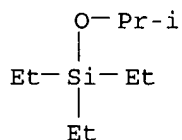
RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

RN 1571-45-5 HCAPLUS

CN Silane, triethyl(1-methylethoxy)- (9CI) (CA INDEX NAME)



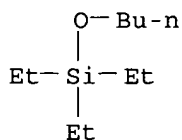
IT 2751-87-3P 51276-59-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

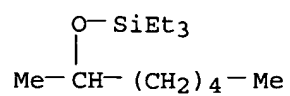
RN 2751-87-3 HCAPLUS

CN Silane, butoxytriethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 51276-59-6 HCAPLUS

CN Silane, triethyl[(1-methylhexyl)oxy]- (9CI) (CA INDEX NAME)



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